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DEPARTMENT OF CIVIL ENGINEERING
AND ENGINEERING MECHANICS

Elasticity, Piezoelectricity and Crystal Lattice Dynamics

by

R. D. Mindlin

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Technical Report No. 24

September, 1972

Elasticity, Piezoelectricity and Crystal Lattice Dynamics

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Abstract — A review of some recent developments in the area between the dynamical theory of crystal lattices, in the harmonic approximation, and the classical, linear theories of elasticity and piezoelectricity.

1. Introduction

The differential equations of the classical theory of the anisotropic, elastic continuum are the long wave, low frequency limit of the finite difference equations of the dynamical theory of crystal lattices of mass particles. Consequently, solutions of the difference equations converge to the corresponding solutions of the differential equations as periods and wave lengths increase. Conversely, the two diverge as periods and wave lengths diminish or, in the case of equilibrium, as dimensions diminish. The discrepancy is even greater between classical piezoelectricity and modern theories of the crystal lattice of polarizable atoms because these two do not even converge at the long wave, low frequency limit. In both cases, the defects are due to insufficient consideration, in the continuum theories, of the structure of crystals and the interactions between atoms or molecules.

During the past dozen years, there has been a revival of activity aimed at extending the range of the classical theories of elasticity and piezoelectricity to account for more aspects of structure and interatomic interactions. Developments have progressed along numerous paths, including: (1) rediscoveries of the early terms and the whole of Cauchy's [1] infinite series representation of an elastic solid with a periodic structure — equivalent to taking into account all of the gradients of strain in the potential energy density; (2) form-

ulation of continuum theories of deformation and polarization of crystals with compound lattice structure; (3) revival and extensions of the Cosserat [2] continuum representation of molecular crystals; (4) augmentation of the classical (Voigt [3]) theory of piezoelectricity to include the contribution of the gradient of the electronic polarization.

Not all of the new developments contribute to reduction of the gap between continuum and lattice theories if they are judged on the grounds that the extended range of the continuum theory must conform to the lattice theory in that range and that the augmented equations must accommodate observed or observable physical phenomena not accounted for by the classical theory. However, the following favorable conclusions can be reached:

(1) The Cauchy-type theories are acceptable if at least the first and second gradients of strain are included. Then the additional terms in the dispersion relation for plane waves can be matched to the early terms of the lattice dispersion relation without sacrificing positive definiteness of the potential energy density; and the phenomenon of surface energy of deformation makes its appearance for centrosymmetric as well as non-centrosymmetric crystals (the latter requiring only the strain and its first gradient).

(2) The continuum equations developed recently for diatomic crystals are the correct, long wave limits of the difference equations of the NaCl-type lattice of both mass particles and polarizable atoms and they give the correct behavior of the optical branches at long wave lengths, accommodate surface energy of deformation (and polarization) and, with the inclusion of the magnetic field, yield a dispersion relation exhibiting the long wave portions of the coupled acoustic, optical and electromagnetic branches.

(3) The equations of the Cosserat continuum are the long wave limit of the difference equations of motion of monomolecular

crystals and contribute the long wave behavior of the soft optical mode. The recent extension of the Cosserat theory to include a micro-structure that is deformable, as well as rotatable, may prove to describe the higher modes.

(4) The addition of the first gradient of the electronic polarization to the energy density in classical piezoelectricity supplies the missing terms required to match the long wave limit of the difference equations of the lattice of polarizable atoms and serves to accommodate several observed phenomena otherwise not included: surface energy of deformation and polarization, anomalous capacitance of thin dielectric films, acoustical activity and, with the inclusion of the magnetic field, optical activity.

In the following pages, typical examples of these developments and results are described within the framework of linear continuum theories (linear differential equations) and lattice theories in the harmonic approximation (linear difference equations). The point of view is from the side of continuum theories and they are t·ated in more general terms than are the lattice theories. For the latter, reference may be made to "Theory of Lattice Dynamics in the Harmonic Approximation" by Maradudin, Montroll, Weiss and Ipatova (Academic Press, 1971).

2. Simple-Cubic Lattice of Mass Points and Classical Elasticity

The fact that the equations of classical elasticity are the long wave, low frequency limit of the difference equations of a lattice of mass particles, indicates that classical elasticity is limited to wave lengths and bodily dimensions large in comparison with the distance between nearest neighbor atoms (the "lattice parameter"). For the actual magnitudes of the errors, it is necessary to compare detailed solutions of analogous problems in the two types of theory. For this purpose, it is convenient to employ, for the lattice equations, those formulated by Gazis, Herman and Wallis [4] for a simple cubic lattice with nearest and next nearest neighbor central force interactions and their novel angular interactions between three, successive, non-collinear atoms. Simple-cubic is the simplest of all lattice structures and the Gazis-Herman-Wallis equations are the simplest, valid, cubic-lattice equations that do not require a relation among the three elastic constants of cubic symmetry Although no natural crystals with simple-cubic structure are known to exist, the equations are suitable for a study of the major effects of wave length and size.

i. Difference Equations.

In rectangular coordinates x_i, $i = 1,2,3$, the atoms of the simple-cubic lattice are taken to be at the points $x_1 = la$, $x_2 = ma$, $x_3 = na$, where l, m, n are positive or negative integers and a is the lattice parameter. The central force constants (i.e., force per unit relative displacement) between nearest neighbor atoms and between next nearest neighbor atoms are designated by α and β, respectively, while γ is the angular force constant between three, successive, non-collinear atoms. The rôles of the three force constants are depicted schematically by dashed lines in Fig. 1.

With $u_i^{\ell,m,n}$, $i=1,2,3$, the rectangular components of displacement of the atom at ℓ, m, n, Gazis, Herman and Wallis [4] find three equations of motion of the type

$$
\begin{aligned}
M\ddot{u}_1^{\ell,m,n} = {} & \alpha\left(u_1^{\ell+1,m,n} + u_1^{\ell-1,m,n} - 2u_1^{\ell,m,n}\right) \\
& + \beta\left(u_1^{\ell+1,m+1,n} + u_1^{\ell-1,m-1,n} + u_1^{\ell+1,m-1,n} + u_1^{\ell-1,m-1,n}\right. \\
& \qquad \left. + u_1^{\ell+1,m,n} + u_1^{\ell-1,m,n-1} + u_1^{\ell+1,m,n-1} + u_1^{\ell-1,m,n+1} - 8u_1^{\ell,m,n}\right) \\
& + (\beta+\gamma)\left(u_2^{\ell+1,m+1,n} + u_2^{\ell-1,m-1,n} - u_2^{\ell+1,m-1,n} - u_2^{\ell-1,m+1,n}\right. \\
& \qquad \left. + u_3^{\ell+1,m,n+1} + u_3^{\ell-1,m,n-1} - u_3^{\ell+1,m,n-1} - u_3^{\ell-1,m,n+1}\right) \\
& + 4\gamma\left(u_1^{\ell,m+1,n} + u_1^{\ell,m-1,n} + u_1^{\ell,m,n+1} + u_1^{\ell,m,n-1} - 4u_1^{\ell,m,n}\right),
\end{aligned}
\tag{2.1}
$$

where M is the mass of the atom. The remaining two equations of motion are obtained by cyclical permutation of subscripts and superscripts. Born and von Kármán, in their classical paper [5], would have found the same equations if they had taken their $\alpha, \beta, \gamma, \delta, \kappa$ to be the present $\alpha, 4\gamma, \delta, 0, \beta+\gamma$, respectively.

At free boundaries $\ell = \pm L$, the conditions to be satisfied are

$$
\begin{aligned}
& \pm\alpha\left(u_1^{\pm(L+1),m,n} - u_1^{\pm L,m,n}\right) \\
& \pm\beta\left(u_1^{\pm(L+1),m+1,n} + u_1^{\pm(L+1),m-1,n} + u_1^{\pm(L+1),m,n+1} + u_1^{\pm(L+1),m,n-1} - 4u_1^{\pm L,m,n}\right) \\
& + \beta\left(u_2^{\pm(L+1),m+1,n} - u_2^{\pm(L+1),m-1,n} + u_3^{\pm(L+1),m,n+1} - u_3^{\pm(L+1),m,n-1}\right) \\
& \pm 2\gamma\left(u_1^{\pm L,m+1,n} + u_1^{\pm L,m-1,n} + u_1^{\pm L,m,n+1} + u_1^{\pm L,m,n-1} - 4u_1^{\pm L,m,n}\right) \\
& + \gamma\left(u_2^{\pm(L+1),m+1,n} - u_2^{\pm(L+1),m-1,n} - u_2^{\pm L,m+1,n} + u_2^{\pm L,m-1,n}\right) \\
& + \gamma\left(u_3^{\pm(L+1),m,n+1} - u_3^{\pm(L+1),m,n-1} - u_3^{\pm L,m,n+1} + u_3^{\pm L,m,n-1}\right) = 0.
\end{aligned}
\tag{2.2}
$$

II. Reduction to Equations of Classical Elasticity.

To show how (2.1) reduces to the corresponding equation in classical elasticity, it is convenient to put it in a different form [6]. Define difference operators as follows:

$$
\begin{aligned}
& \Delta_1^+ u_i^{\ell,m,n} = \left(u_i^{\ell+1,m,n} - u_i^{\ell,m,n}\right)/a, \quad \Delta_1^- u_i^{\ell,m,n} = \left(u_i^{\ell,m,n} - u_i^{\ell-1,m,n}\right)/a, \\
& \Delta_1^2 u_i^{\ell,m,n} = \Delta_1^+ \Delta_1^- u_i^{\ell,m,n} = \left(u_i^{\ell+1,m,n} - 2u_i^{\ell,m,n} + u_i^{\ell-1,m,n}\right)/a^2, \\
& \Delta_1 \Delta_2 u_i^{\ell,m,n} = \tfrac{1}{4}\left(\Delta_1^+\Delta_2^+ + \Delta_1^-\Delta_2^- + \Delta_1^+\Delta_2^- + \Delta_1^-\Delta_2^+\right) u_i^{\ell,m,n}
\end{aligned}
\tag{2.3}
$$

and analogous definitions, e.g. $\Delta_2^+ u_i^{\ell,m,n} = (u_i^{\ell,m+1,n} - u_i^{\ell,m,n})/a$, for forward, backward, second central and cross differences in the remaining coordinate directions. Then, noting that

$$\begin{aligned} u_i^{\ell+1,m+1,n} + u_i^{\ell-1,m-1,n} + u_i^{\ell+1,m-1,n} + u_i^{\ell-1,m+1,n} - 4u_i^{\ell,m,n} &= a^2(a^2\Delta_1^2\Delta_2^2 + 2\Delta_1^2 + 2\Delta_2^2)u_i^{\ell,m,n}, \\ u_i^{\ell+1,m+1,n} + u_i^{\ell-1,m-1,n} - u_i^{\ell+1,m-1,n} - u_i^{\ell-1,m+1,n} &= 4a^2\Delta_1\Delta_2 u_i^{\ell,m,n}, \end{aligned} \tag{2.4}$$

we can write (2.1) in the form

$$\rho\ddot{u}_1^{\ell,m,n} = [c_{11}\Delta_1^2 + c_{44}(\Delta_2^2+\Delta_3^2) + \tfrac{1}{2}a^2c_{12}\Delta_1^2(\Delta_2^2+\Delta_3^2)]u_1^{\ell,m,n} + (c_{12}+c_{44})(\Delta_1\Delta_2 u_2^{\ell,m,n} + \Delta_1\Delta_3 u_3^{\ell,m,n}), \tag{2.5}$$

where

$$\rho = M/a^3, \quad ac_{11} = \alpha + 4\beta, \quad ac_{12} = 2\beta, \quad ac_{44} = 2(\beta + 2\gamma). \tag{2.6}$$

Now, expand the difference operators, on $u_i^{\ell,m,n}$, in Taylor series of partial derivatives $\partial_i = \partial/\partial x_i$, of continuous displacement functions $u_i(x_i)$ [7]:

$$\begin{aligned} \Delta_i^2 u_j^{\ell,m,n} &= (1 + \tfrac{1}{12}a^2\partial_i^2 + \cdots)\partial_i^2 u_j, \\ \Delta_i\Delta_j u_k^{\ell,m,n} &= (1 + \tfrac{1}{6}a^2\partial_i^2 + \tfrac{1}{6}a^2\partial_j^2 + \cdots)\partial_i\partial_j u_k, \\ \Delta_i^2\Delta_j^2 u_k^{\ell,m,n} &= (1 + \tfrac{1}{12}a^2\partial_i^2 + \tfrac{1}{12}a^2\partial_j^2 + \cdots)\partial_i^2\partial_j^2 u_k. \end{aligned} \tag{2.7}$$

If only second derivatives are retained, (2.5) reduces to

$$\rho\ddot{u}_1 = [c_{11}\partial_1^2 + c_{44}(\partial_2^2 + \partial_3^2)]u_1 + (c_{12}+c_{44})(\partial_1\partial_2 u_2 + \partial_1\partial_3 u_3), \tag{2.8}$$

which is the equation of motion of classical elasticity for materials with the constants c_{11}, c_{12}, c_{44} of cubic symmetry.

iii. Dispersion Relations.

The designation "long wave, low frequency limit", for (2.8), stems from a comparison of dispersion relations (frequency vs. wave number) for plane waves from (2.5) and (2.8). Consider, for example, longitudinal waves in the x_1-direction. For (2.5), we set

$$u_2^{\ell,m,n} = u_3^{\ell,m,n} = 0, \quad u_1^{\ell,m,n} = Ae^{i(\xi\ell a - \omega t)}, \quad 0 < \xi a < \pi. \tag{2.9}$$

Then (2.5) is satisfied if

$$\omega = \frac{2}{a}\sqrt{\frac{c_{11}}{\rho}}\ \sin\frac{\xi a}{2}\,. \tag{2.10}$$

For (2.8), we set

$$u_2 = u_3 = 0, \quad u_1 = A e^{i(\xi x_1 - \omega t)} \tag{2.11}$$

and find

$$\omega = \xi\sqrt{\frac{c_{11}}{\rho}}\,. \tag{2.12}$$

The two dispersion relations, (2.10) and (2.12), are illustrated in Fig. 2. It may be seen that the lattice dispersion relation (2.10) approaches the continuum relation (2.12) as the wave length approaches infinity, i.e. as the wave number, ξ, approaches zero. Simultaneously, the frequency, in a monatomic Bravais lattice, also approaches zero.

For more detailed examinations of the differences between solutions of lattice and continuum equations, it is necessary to consider problems for bodies with at least one finite dimension with which to compare the lattice parameter a.

iv. Thickness-Shear Vibrations of a Plate [8].

In a plate bounded by $\ell = \pm L$, consider the displacements

$$u_1^{\ell,m,n} = u_2^{\ell,m,n} = 0, \quad u_3^{\ell,m,n} = (A_1 \cos\xi\ell a + A_2 \sin\xi\ell a)e^{i\omega t}, \quad 0 \le \xi a \le \pi. \tag{2.13}$$

With these displacements, the first two equations of the type (2.5) are satisfied identically and the third is satisfied if

$$\rho a^2\omega^2 = 4c_{44}\sin^2\tfrac{1}{2}\xi a\,. \tag{2.14}$$

Upon substituting the displacements (2.13) in the boundary conditions (2.2), we find that the first two conditions are satisfied identically and the third is satisfied if

$$\xi a = p\pi/(2L+1), \quad p = 0,1,2,\ldots < 2L+1, \tag{2.15}$$

where even and odd p apply to symmetric and antisymmetric modes, respectively. From (2.14) and (2.15), the frequencies are

$$\omega = \frac{2}{a}\left(\frac{c_{44}}{\rho}\right)^{1/2} \sin\frac{p\pi}{2(2L+1)} \quad , \quad p = 0, 1, 2, \ldots < 2L+1 \tag{2.16}$$

and the displacements, from (2.13) and (2.15), are

$$u_3^{\ell,m,n} = \left(A_1 \cos\frac{p\pi\ell}{2L+1} + A_2 \sin\frac{p\pi\ell}{2L+1}\right) e^{i\omega t} . \tag{2.17}$$

To compare the lattice solution with the continuum one, we consider a continuum plate of thickness $2h$, where

$$2h = (2L+1)a , \tag{2.18}$$

i.e. each layer of atoms is replaced by a thickness a of the continuum. The frequencies of the thickness-shear modes of such a plate are given by

$$\omega = \frac{p\pi}{2h}\cdot\left(\frac{c_{44}}{\rho}\right)^{1/2} , \quad p = 0, 1, 2 \ldots \tag{2.19}$$

and the displacements are

$$u_3 = \left(A_1 \cos\frac{p\pi x_1}{2h} + A_2 \sin\frac{p\pi x_1}{2h}\right) e^{i\omega t} . \tag{2.20}$$

In the long wave, low frequency approximation,

$$\ell a \to x_1 , \quad p \ll 2L+1 , \tag{2.21}$$

in which case (2.16) and (2.17) approach (2.19) and (2.20), respectively.

If the frequency of the lowest, antisymmetric, thickness-shear mode in the continuum plate, i.e $p=1$ in (2.19), is used as a reference frequency ω_1:

$$\omega_1 = \frac{\pi}{2h}\left(\frac{c_{44}}{\rho}\right)^{1/2} = \frac{\pi}{(2L+1)a}\left(\frac{c_{44}}{\rho}\right)^{1/2} , \tag{2.22}$$

the normalized frequencies for the lattice are

$$\Omega = \frac{\omega}{\omega_1} = \frac{2(2L+1)}{\pi}\sin\frac{p\pi}{2(2L+1)}, \quad p = 0,1,2,\ldots < 2L+1, \tag{2.23}$$

and these are to be compared with the normalized frequencies, $p = 0,1,2\ldots$ for the continuum.

The discrepancy between the frequencies p and Ω and the corresponding departure of the lattice mode shape from the sinusoidal form characteristic of the continuum, as the order of the mode increases, are illustrated in Fig. 3 for the case of fifteen layers. It may be seen that, for the first few modes, where the lattice mode shapes are nearly sinusoidal, the normalized frequencies p and Ω are nearly the same. Inspection of the case $p=3$ shows that the half wave length can be as small as five lattice parameters with a good representation of the mode shape by a sinusoid and an error in frequency of less than 2%. However, as the mode shape departs from the sinusoidal for increasing orders, the frequencies p and Ω separate — by almost 50% for the highest mode, in the case of fifteen layers. As the number of layers increases, the percent discrepancy between the frequencies of the highest lattice mode and the corresponding continuum mode approaches $50\pi - 100 = 57\%$.

It should be noted that, whereas the number of modes in the continuum plate is unlimited, the number of modes in the lattice plate is equal to the number of layers. This is because a wave described by N points can have no more than N-1 nodes.

V. Face-Shear and Thickness-Twist waves in a plate [8].

Waves, in a plate, with displacement and wave normal at right angles to each other and parallel to the faces of the plate, are called thickness-twist waves except for the wave of zero order (in which the displacement does not vary through the thickness of the plate) which is called a face-shear wave. In the continuum, these waves are special cases of Love's [9] transverse waves in a superficial layer

In the lattice plate, the waves are represented by displacements of the form

$$u_1^{\ell,m,n} = u_2^{\ell,m,n} = 0, \quad u_3^{\ell,m,n} = (A_1 \cos\xi\ell a + A_2 \sin\xi\ell a)e^{i(\eta m a - \omega t)}, \tag{2.24}$$

where $0 \leq \xi a \leq \pi$, $0 \leq \eta a \leq \pi$. This time, the equations of motion of the type (2.3) require

$$\rho a^2 \omega^2 = 4 c_{44}(\sin^2 \tfrac{1}{2}\xi a + \sin^2 \tfrac{1}{2}\eta a) \tag{2.25}$$

and the boundary conditions (2.2) again require (2.15). Thus, the normalized frequencies are

$$\Omega = \frac{\omega}{\omega_1} = \frac{2(2L+1)}{\pi}\left(\sin^2 \frac{p\pi}{2(2L+1)} + \sin^2 \tfrac{1}{2}\eta a\right)^{1/2}, \quad p = 0, 1, 2 \ldots < 2L+1, \tag{2.26}$$

and the displacements are

$$u_3^{\ell,m,n} = \left(A_1 \cos\frac{p\pi\ell}{2L+1} + A_2 \sin\frac{p\pi\ell}{2L+1}\right)e^{i(\eta m a - \omega t)}. \tag{2.27}$$

In the long wave, low frequency limit $(\ell a \to x_1, ma \to x_2, p \ll 2L+1)$ these become the known results for the special case of Love waves [9]:

$$\Omega = [p^2 + (2\eta h/\pi)]^{1/2}, \quad p = 0, 1, 2 \ldots \tag{2.28}$$

$$u_3 = [A_1 \cos(p\pi x_1/2h) + A_2 \sin(p\pi x_1/2h)]e^{i(\eta x_2 - \omega t)}. \tag{2.29}$$

The real branches of the dispersion relation (2.26) are illustrated in Fig. 4 for a plate fifteen layers thick (L = 7). At infinite wave length ($\eta = 0$) along the plate, the mode reduce to the thickness-shear modes illustrated in Fig. 3. These variations of displacement across the thickness of the plate are maintained for all wavelengths, $2\pi/\eta$, along the plate. The major differences between the dispersion relations for the lattice and the continuum are: each of the finite number, 2L+1, of branches of the lattice dispersion relation (2.26) has a high frequency cut off, in addition to a low

frequency cut-off (2.23), and all have the same upper cut-off of wave number, $\eta = \pi/a$, i.e wave length equal to $2a$; whereas all the infinity of real branches of the continuum dispersion relation (2.28) are hyperbolic curves extending from low frequency cut-offs $\Omega = 1, 2, \ldots, \infty$, at $\eta = 0$, to infinite frequencies and wave numbers — asymptotic to

$$\Omega = (2L+1)\eta a/\pi, \tag{2.30}$$

which is the straight line starting from the lower left corner and passing through the upper right corner of Fig. 4 and is, in fact, the face shear branch of the continuum dispersion relation. Thus, the dispersion relation for the continuum is a good approximation to that of the lattice only in the lower left region of Fig. 4; i.e. for long wave lengths, in comparison with a, both along the plate and across its thickness. Two or three times a is sufficient for accuracy within 2%.

As in the case of the continuum, the lattice dispersion relation has branches for real frequency and imaginary wave number which are not shown in Fig. 4.

The problem of face-shear and thickness-shear waves in a plate has also been solved for the face-centered cubic lattice (Brady [10]) and for the body centered cubic lattice (Gong [11]).

vi. Torsional Equilibrium of a Rectangular Bar.

The bar is bounded by free faces at $\ell = \pm L$ and $m = \pm M$ and is in equilibrium under a twist about the axis of x_3 with angle of twist τ per unit length.

By analogy with the St. Venant solution of the equations of classical elasticity for the analogous problem [12], it is assumed that

$$\begin{aligned} u_1^{\ell,m,n} &= -\tau a^2 mn, \\ u_2^{\ell,m,n} &= \tau a^2 \ell n, \\ u_3^{\ell,m,n} &= \tau a^2(\ell m + A \sin \ell\theta \sinh m\varphi); \quad 0 < \theta < \pi. \end{aligned} \tag{2.31}$$

With these displacements, the first two equations of the type (2.5), with the left hand side zero, are satisfied identically and the third equation is satisfied if

$$\cosh\varphi = 2 - \cos\theta . \tag{2.32}$$

The conditions of the type (2.2), for free boundaries, reduce, in view of (2.31), to

$$\pm 2\left(u_3^{\pm(L+1),m,n} - u_3^{\pm L,m,n}\right) + u_1^{\ell,m,n+1} - u_1^{\ell,m,n-1} = 0 \quad \text{on} \quad \ell = \pm L, \tag{2.33}$$

$$\pm 2\left(u_3^{\ell,\pm(M+1),n} - u_3^{\ell,\pm M,n}\right) + u_2^{\ell,m,n+1} - u_2^{\ell,m,n-1} = 0 \quad \text{on} \quad m = \pm M. \tag{2.34}$$

Upon substituting (2.31) in (2.33), we find

$$\theta = \theta_p = (2p-1)\pi/(2L+1), \quad p = 1, 2, \ldots, L. \tag{2.35}$$

Hence, the third of (2.31) may be written as a finite series:

$$u_3^{\ell,m,n} = \tau a^2\left(\ell m + \sum_{p=1}^{p=L} A_p \sin \ell\theta_p \sinh m\varphi_p\right). \tag{2.36}$$

Substitution of (2.36) in the boundary conditions (2.34) yields

$$\sum_{p=1}^{p=L} A_p \sin \ell\theta_p \sinh \tfrac{1}{2}\varphi_p \cosh(M+\tfrac{1}{2})\varphi_p = -\ell; \quad \ell = 1, 2, \ldots, L, \tag{2.37}$$

i.e. a set of L simultaneous, linear, algebraic equations on the coefficients A_p. The system of equations can be solved explicitly for the A_p by a method analogous to that for determining Fourier coefficients. Multiply both sides of (2.37) by $\sin \ell\theta_q$ and sum over ℓ from $\ell = 1$ to $\ell = L$. Now [13],

$$\sum_{\ell=1}^{\ell=L} \ell \sin \ell\theta_p = \frac{\sin L\theta_p}{4\sin^2 \frac{1}{2}\theta_p} - \frac{L\cos(L+\frac{1}{2})\theta_p}{2\sin\frac{1}{2}\theta_p}. \tag{2.38}$$

Also, employing (2.35), we find

$$\sum_{\ell=1}^{\ell=L} \sin \ell\theta_p \sin \ell\theta_q = \begin{cases} 0, & q \neq p \\ \frac{1}{4}(2L+1), & q = p. \end{cases} \tag{2.39}$$

Hence,

$$A_p = \frac{2L \sin \frac{1}{2}\theta_p \cos (L+\frac{1}{2})\theta_p - \sin L\theta_p}{(2L+1)\sinh^3 \frac{1}{2}\varphi_p \cosh (M+\frac{1}{2})\varphi_p} . \tag{2.40}$$

Substitution of (2.40) in (2.36) completes the solution for the warping function $u_3^{\ell,m,n}$. The results are shown in Fig. 5 in which the ratios of integers at the lattice points give $u_3^{\ell,m,n}/\tau a^2$ at those points. Fig. 5 is to be compared with Fig. 6 which depicts typical contours of the warping functions for square and long rectangular sections from the St. Venant solution. It may be seen that, with one side of the cross section restricted to three atoms ($L = 1$), the warping bears little resemblance to that found by St. Venant; namely, there is no warping of the square section ($L=1$, $M=1$) and, in each succeeding section ($L=1$, $M = 2, 3, 4$), the displacements at a long side ($\ell = \pm 1$, $m = 0, \pm 1, \pm 2, \ldots$) do not have a maximum and a minimum between the center and the ends, as they have in the continuum solution. However, if the smaller dimension is increased to five atoms ($L = 2$, $M = 2, 3, \ldots$) the dissimilarity disappears For the square ($L=2$, $M=2$), it may be seen that the cross section is divided into eight sectors, with alternating signs of displacements, instead of the usual four sectors for long rectangular sections. This is precisely the result found by St. Venant for the continuum, as illustrated in Fig. 6. For the rectangular sections $L=2$, $M=3$ and $L=2$, $M=4$, the displacements along a long side reach a maximum and a minimum, near the ends, while, along a short side, the displacements vary monotonically. Again, these results are the same as the corresponding ones in St. Venant's solution, as illustrated in Fig. 6. Thus, the cross section need have only as many as five atoms along the shorter side for the displacements to have the major qualitative properties found in the continuum solution.

3. Strain Gradient Theories

Extensions of classical elasticity to account for crystal structure began in 1851 with Cauchy's [1] infinite series representation of an isotropic material with a periodic structure. Although Cauchy did not carry his idea very far, it is now known that his theory corresponds to an infinite series expansion of difference operators, in a lattice theory, in terms of differential operators; or, equivalently, augmentation of classical elasticity through the inclusion of all the gradients of strain in the potential energy density. Little attention was paid to the work for many years— possibly due to the complexity introduced by Cauchy's consideration of non-centrosymmetric isotropy; possibly due to an error of omission in the constitutive equation for the symmetric part of the stress; possibly due to Todhunter's assessment: "This consists merely of generalities, and is apparently of no importance" [12, Vol. I, p. 374].

i. Rotation Gradient.

Interest in the gradient type of theory was stimulated, in 1960, by Aero and Kuvshinskii [14], Grioli [15], Rajagopal [16] and Truesdell and Toupin [17] who took into account the first gradient of the rotation:

$$\kappa_{ij} = \tfrac{1}{2}\,\delta_{jk\ell}\,\partial_i\partial_k u_\ell\,, \tag{3.1}$$

where δ_{ijk} is the unit alternating tensor:

$$\delta_{ijk} = \begin{cases} +1, & ijk = 123, 231, 312, \\ -1, & ijk = 321, 213, 132, \\ 0, & \text{otherwise}. \end{cases} \tag{3.2}$$

A connection with crystal lattice theory was noted by Krumhansl [18], in 1963, who showed, by expansion of the differences in the expression for the potential energy of a general Bravais lattice, that the second order terms, in the resulting series of derivatives, contain the rotation gradient

The novel features accompanying the rotation gradient are the

appearances of an antisymmetric part of the stress (indeterminate), a couple stress and a material constant with the dimension of length; but, except for a tenuous connection with molecular crystals (see Article 5), no relation to crystal lattice theory appears to have been established beyond Krumhansl's brief remark.

ii First Strain Gradient.

The rotation gradient has eight independent components which are eight of the eighteen components of the first gradient of the strain. The additional ten components are

$$\tfrac{1}{3}\left(\partial_i\partial_j u_k + \partial_j\partial_k u_i + \partial_k\partial_i u_j\right). \tag{3.3}$$

Alternatively, in terms of the strain,

$$S_{ij} = \tfrac{1}{2}\left(\partial_i u_j + \partial_j u_i\right), \tag{3.4}$$

all eighteen components may be expressed as $\partial_i S_{jk}$; but perhaps the simplest form is the second gradient of the displacement:

$$S_{ijk} = \partial_i\partial_j u_k . \tag{3.5}$$

The fundamental equations for the elastic material in which account is taken of the full first gradient of the strain were given by Toupin [19] in 1962. In the linear case, the potential energy density may be expressed in the form

$$W = c_{ijk}S_{ijk} + \tfrac{1}{2}c_{ijkl}S_{ij}S_{kl} + \tfrac{1}{2}c_{ijklmn}S_{ijk}S_{lmn} + c_{ijklm}S_{ij}S_{klm}, \tag{3.6}$$

where the $c_{ij\ldots}$ are material constants. The most interesting feature of (3.6) is the linear term $c_{ijk}S_{ijk}$ which corresponds to a self-equilibrating initial stress and gives rise to a surface energy of deformation: an observed physical phenomenon not contained in classical elasticity.

The surface energy of deformation is a part of the energy associated with the separation along a surface. Part of the separation energy is the bond energy — that required to break the atomic bonds across the surface while the

relative positions of the atoms in each of the two resulting portions are held fixed -- say, by fictitious forces. The release of these forces is accompanied by a deformation, localized near the surfaces, and an associated (negative) energy: the surface energy of deformation — estimates of the magnitude of which range as high as 40% of the bond energy [20]. The extreme localization of deformation at the surface was first observed in 1961 by Germer, MacRae and Hartman [21] by means of low energy electron diffraction measurements at nickel surfaces. They found that the displacement of the superficial layer of atoms toward the interior was five times as large as that of the next layer. Toupin and Gazis [22], in 1963, found mathematical solutions for a similar surface deformation within the framework of Toupin's strain gradient equations and also exhibited the correspondence with a one-dimensional, monatomic lattice with nearest and next nearest neighbor interactions.

The first strain gradient theory, however, suffers from two deficiencies. First of all, it contains a surface energy of deformation only for non-centrosymmetric materials. This is evidenced by the third rank tensor coefficient of the linear term in (3.6); whereas the elasticity of centrosymmetric materials can be characterized only by tensors of even rank. Secondly, the dispersion relation for plane waves can match that for a lattice beyond the linear range only if the requirement of a positive strain energy density is abandoned - as shown in the following section. Both of these defects disappear if the second gradient of the strain is included.

iii. Second Strain Gradient [23].

If the strain and its first two gradients are taken into account, the potential energy density for a centrosymmetric material has the form

$$W = \tfrac{1}{2} c_{ijkl} S_{ij} S_{kl} + \tfrac{1}{2} a_{ijklmn} S_{ijk} S_{lmn} + \tfrac{1}{2} \beta_{ijklmnpq} S_{ijkl} S_{mnpq} + \gamma_{ijklmn} S_{ij} S_{klmn} + \beta^{o}_{ijkl} S_{ijkl}, \tag{3.7}$$

where, in addition to (3.4) and (3.5),

$$S_{ijkl} = \partial_i \partial_j \partial_k u_l . \tag{3.8}$$

This energy and the usual kinetic energy density $\frac{1}{2}\rho \dot{u}_i \dot{u}_i$ lead to the stress equations of motion

$$\partial_i T_{il} - \partial_i \partial_j T_{ijl} + \partial_i \partial_j \partial_k T_{ijkl} = \rho \ddot{u}_l , \tag{3.9}$$

where the stresses T_{ij}, T_{ijk} and T_{ijkl} are given by

$$\begin{aligned} T_{ij} &= \partial W/\partial S_{ij} = c_{ijkl} S_{kl} + \gamma_{ijklmn} S_{klmn} , \\ T_{ijk} &= \partial W/\partial S_{ijk} = \alpha_{ijklmn} S_{lmn} , \\ T_{ijkl} &= \partial W/\partial S_{ijkl} = \gamma_{ijklmn} S_{mn} + \beta_{ijklmnpq} S_{mnpq} + \beta^{\circ}_{ijkl} , \end{aligned} \tag{3.10}$$

and to three, vector boundary tractions:

$$\begin{aligned} t^{(1)}_l &= n_i (T_{il} - \partial_j T_{ijl} + \partial_j \partial_k T_{ijkl}) + L_i [n_j (T_{ijl} - \partial_k T_{ijkl})] + L_i L_j (n_k T_{ijkl}) \\ &\quad - L_i [(\delta_{ip} - n_i n_p)(\partial_p n_q) n_j n_k T_{ijkl}] , \\ t^{(2)}_l &= n_i n_j (T_{ijl} - \partial_k T_{ijkl}) + n_i L_j (n_k T_{ijkl}) + L_k (n_i n_j T_{ijkl}) , \\ t^{(3)} &= n_i n_j n_k T_{ijkl} , \end{aligned} \tag{3.11}$$

where

$$L_i = n_i (\delta_{jk} - n_j n_k) \partial_k n_j - (\delta_{ij} - n_i n_j) \partial_j \tag{3.12}$$

It will be observed that the strain energy density (3.7) has no term linear in S_{ij}. This is because, just as in classical elasticity, the material configuration, to which W is referred, can be chosen so that such a term does not appear. Also, there is no term in (3.7) linear in S_{ijk} as its material coefficient would be a tensor of odd rank, which cannot exist for centrosymmetric materials. This leaves the only linear term to be the one in S_{ijkl}, which can be shown to produce a surface energy of deformation, as follows.

From an unstrained body under no external forces, remove a portion, of volume V, bounded by a surface S. The energy in such a portion, in equilibrium under no external forces, is

$$\mathcal{W} = \int_V W \, dV , \tag{3.13}$$

or, from (3.7) and (3.10),

$$\mathcal{W} = \frac{1}{2}\int_V \left(T_{ij}S_{ij} + T_{ijk}S_{ijk} + T_{ijkl}S_{ijkl}\right)dV + \frac{1}{2}\int_V \beta^{\circ}_{ijkl}S_{ijkl}\,dV. \tag{3.14}$$

The second integral in (3.14) enters because, as may be seen in (3.10), it corresponds to a constant term β°_{ijkl} in T_{ijkl} whereas the remaining parts of T_{ij}, T_{ijk} and T_{ijkl} vary in proportion to the strain and its gradients. The first integral in (3.14) can be transformed to

$$\frac{1}{2}\int_S \left[t^{(1)}_i u_i + t^{(2)}_i (n_j\partial_j)u_i + t^{(3)}_i (n_j\partial_j)^2 u_i\right]dS, \tag{3.15}$$

which vanishes since the surface S is free of traction. This leaves

$$\mathcal{W} = \frac{1}{2}\int_V \beta^{\circ}_{ijkl}S_{ijkl}\,dV = \frac{1}{2}\int_S n_i\beta^{\circ}_{ijkl}\partial_j\partial_k u_l\,dS \tag{3.16}$$

as an energy that remains in V although the body is under no external forces. The energy per unit area of the surface is, from (3.16),

$$W^S = \frac{1}{2}n_i\beta^{\circ}_{ijkl}\partial_j\partial_k u_l\Big]_S . \tag{3.17}$$

To show that this energy is localized near the surface, it is sufficient to consider the case of the half-space $x_1 \geq 0$ with $x_1 = 0$ free of traction. Assume

$$u_1 = u(x_1), \quad u_2 = u_3 = 0. \tag{3.18}$$

Then the stress equations of equilibrium, from (3.9), reduce to

$$\partial_1 T_{11} - \partial_1^2 T_{111} + \partial_1^3 T_{1111} = 0, \tag{3.19}$$

while the boundary conditions, from (3.11), become

$$T_{11} - \partial_1 T_{111} + \partial_1^2 T_{1111} = 0, \quad T_{111} - \partial_1 T_{1111} = 0, \quad T_{1111} = 0 \quad \text{on } x_1 = 0. \tag{3.20}$$

Also, with the assumed form of displacements (3.18), the constitutive equations (3.10) take the form

$$T_{11} = c\,\partial_1 u_1 + \gamma\,\partial_1^3 u_1, \quad T_{111} = \alpha\,\partial_1^2 u_1, \quad T_{1111} = \beta_0 + \gamma\,\partial_1 u_1 + \beta\,\partial_1^3 u_1 \tag{3.21}$$

and the surface energy per unit area (3.17) becomes, after noting that $n_1 = -1$ and $\overset{\circ}{\beta}_{ijks} = \beta_0$,

$$W^s = -\tfrac{1}{2}\beta_0\, \partial_1^2 u_1\Big]_{x_1=0}\,. \tag{3.22}$$

Substitution of (3.21) in (3.19) gives the displacement equation of equilibrium

$$[c-(\alpha-2\gamma)\partial_1^2+\beta\partial_1^4]\partial_1^2 u_1 = 0, \tag{3.23}$$

or

$$(1-\ell_1^2\partial_1^2)(1-\ell_2^2\partial_1^2)\partial_1^2 u_1 = 0, \tag{3.24}$$

where

$$2c\,\ell_i^2 = \alpha-2\gamma \pm [(\alpha-2\gamma)^2-4\beta c]^{1/2}\,,\quad i=1,2\,. \tag{3.25}$$

Regarding boundary conditions, it may be seen that the first of (3.20) is automatically satisfied if the stress equation of equilibrium (3.19) is satisfied. The remaining two boundary conditions, from (3.20) and (3.21), are

$$[(\alpha-\gamma)\partial_1^2 u_1-\beta\partial_1^4 u_1]_{x_1=0} = 0, \qquad (\gamma\,\partial_1 u_1+\beta\partial_1^3 u_1)_{x_1=0} = -\beta_0\,. \tag{3.26}$$

The solution of (3.24), vanishing at infinity, is

$$u_1 = A_1 e^{-x_1/\ell_1} + A_2 e^{-x_1/\ell_2}\,. \tag{3.27}$$

The values of A_1 and A_2 may be determined from the boundary conditions (3.26) and then the surface energy of deformation is, from (3.22),

$$W^s = -\tfrac{1}{2}\beta_0(A_1\ell_1^{-2}+A_2\ell_2^{-2}). \tag{3.28}$$

The associated strain diminishes exponentially into the interior with decay rate controlled by the magnitude of ℓ_1 and ℓ_2. The appearance of material constants ℓ, with the dimension of length, is typical of the gradient type theories and yields a length scale characteristic of the structure of the material. Such a scale is absent in classical elasticity. An estimate of the order of magnitude of the length scale may be obtained from the electron diffraction measurements at nickel surfaces by Germer, MacRae

and Hartman [21]. Their finding that the displacement of the superficial layer of atoms is five times as large as that of the next layer would lead, on the assumption of a simple exponential decay $e^{-x/\ell}$, to an ℓ of about five eighths of the distance between adjacent layers of atoms. Thus, the deformation is significant only at the first few layers.

Upon departure into the interior, the displacement need not maintain the same sign. The conditions for positive strain energy density do not include relations between α and δ or between α and γ. Hence, from (3.25), the ℓ_i may be complex, corresponding to an oscillating decay of displacement into the interior.

To obtain the corresponding solution for a lattice, consider a single row of particles distributed along the x_1-axis, at unit distance apart, with interactions as far as third neighbors and including self-equilibrating initial forces. Now, separate the lattice between the particles at $n=0$ and $n=-1$ and consider the semi-infinite lattice $n\geq 0$. The separation is effected by the addition of forces P_0, P_1, P_2 on particles at $0, 1, 2$, respectively, equal and opposite to the resultants of the initial forces exerted on those particles by the particles at $-1, -2, -3$. Since the initial forces are self-equilibrating,

$$P_0 + P_1 + P_2 = 0. \tag{3.29}$$

With force constants $\alpha_1, \alpha_2, \alpha_3$ for the interactions between first, second and third neighbors, respectively, and with u_n the displacement of the n^{th} particle, the equilibrium of that particle is expressed by

$$\sum_{i=1}^{i=3} \alpha_i (u_{n+i} - 2u_n + u_{n-i}) = 0, \quad n \geq 3 \tag{3.30}$$

$$\begin{aligned}
\sum_{i=1}^{i=2} \alpha_i (u_{2+i} - 2u_2 + u_{2-i}) + \alpha_3 (u_5 - u_2) &= P_2, \quad n=2, \\
\alpha_1 (u_2 - 2u_1 + u_0) + \alpha_2 (u_3 - u_1) + \alpha_3 (u_4 - u_1) &= P_1, \quad n=1, \\
\alpha_1 (u_1 - u_0) + \alpha_2 (u_2 - u_0) + \alpha_3 (u_3 - u_0) &= P_0, \quad n=0.
\end{aligned} \tag{3.31}$$

We adopt the notations $\Delta u_n = u_{n+1} - u_n$,

$$\Delta^2 u_n = u_{n+1} - 2u_n + u_{n-1}, \quad \Delta^4 u_n = u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2}. \tag{3.32}$$

Then, with

$$\beta_1 = \alpha_1 + 4\alpha_2 + 9\alpha_3, \quad \beta_2 = -\alpha_2 - 6\alpha_3, \quad \beta_3 = \alpha_3; \tag{3.33}$$

the general equation of equilibrium (3.30) becomes

$$(\beta_1 - \beta_2 \Delta^2 + \beta_3 \Delta^4)\Delta^2 u_n = 0, \tag{3.34}$$

or

$$(1 - \lambda_1^2 \Delta^2)(1 - \lambda_2^2 \Delta^2)\Delta^2 u_n = 0, \tag{3.35}$$

where

$$2\beta_1 \lambda_i^2 = \beta_2 \pm (\beta_2^2 + 4\beta_1\beta_3)^{1/2}, \quad i = 1, 2. \tag{3.36}$$

The solution of (3.35), vanishing at infinity, is

$$u_n = A_1 e^{-n\theta_1} + A_2 e^{-n\theta_2} \tag{3.37}$$

provided that

$$\theta_i = \operatorname{arccosh}(1 + 1/2\lambda_i^2), \quad i = 1, 2. \tag{3.38}$$

As for the boundary conditions, there are three for the two constants A_1 and A_2, just as in the case of the continuum solution. Following Gazis and Wallis [24], we sum the three equations (3.31) to obtain

$$(1 - \lambda_1^2 \Delta^2)(1 - \lambda_2^2 \Delta^2)\Delta u_2 = 0, \tag{3.39}$$

which is satisfied identically by the solution (3.37) with (3.38). Thus, as in the case of the continuum, the general condition of equilibrium disposes of one of the three boundary conditions. The remaining two conditions serve to determine A_1 and A_2.

The similarity in form between the differential equations, boundary conditions and solutions for the continuum and the lattice is to be remarked and the correspondence of the continuum expressions to the

long wave wave behavior in the case of the lattice may be verified by noting that

$$\Delta^2 u_n = \partial_1^2 u_1 + \frac{1}{12}\partial_1^4 u_1 + \frac{1}{360}\partial_1^6 u_1 + \cdots$$
$$\Delta^4 u_n = \partial_1^4 u_1 + \frac{1}{6}\partial_1^6 u_1 + \cdots \qquad (3.40)$$
$$\Delta^6 u_n = \partial_1^6 u_1 + \cdots$$

and, in (3.38),

$$g_i \rightarrow 1/\lambda_i . \qquad (3.41)$$

It is also necessary to compare the long wave behavior of the dispersion relations for the continuum and the lattice. The one-dimensional equations of motion, for the two cases, are: for the continuum, from (3.23),

$$[c - (\alpha - 2\gamma)\partial_1^2 + \beta\partial_1^4]\partial_1^2 u_1 = \rho\ddot{u}_1 \qquad (3.42)$$

and, for the lattice, from (3.34),

$$(\beta_1 - \beta_2\Delta^2 + \beta_3\Delta^4)\Delta^2 u_n = M\ddot{u}_n . \qquad (3.43)$$

Inserting the wave forms

$$u_1 = Ae^{i(\xi x_1 - \omega t)}, \qquad u_n = Ae^{i(n\theta - \omega t)}, \qquad (3.44)$$

respectively, we find, to the fourth power of the wave number,

$$\rho\omega^2 = c\xi^2 + (\alpha - 2\gamma)\xi^4 + \cdots , \qquad (3.45)$$
$$M\omega^2 = \beta_1\theta^2 - (\tfrac{1}{2}\beta_1 + \beta_2)\theta^4 + \cdots . \qquad (3.46)$$

If only the strain and its first gradient were considered, (3.45) would be

$$\rho\omega^2 = c\xi^2 + \alpha\xi^4$$

and α is required to be positive by the condition of positive definiteness of the energy density. Hence, in the first gradient theory, the group velocity, $d\omega/d\xi$, must increase as the wave number increases from zero; but, in the lattice the opposite is generally true, as illustrated

in Fig. 7. In the second gradient theory, α is replaced by $\alpha - 2\gamma$ as the coefficient of the second term in the dispersion relation; and the conditions of positive definiteness place no restrictions on the relation between α and γ, so that the group velocities may either increase or decrease with increasing wave number.

4. Diatomic Crystals and Compound Continua

If the lattice structure of a crystal is a simple one of the Bravais type, with one atom per cell, there is no distinction between the long wave limit and the long wave, low frequency limit of the finite difference equations of motion or the dispersion relation. However, if the lattice has a "basis", i.e. a group of two or more atoms per cell, there are high frequency "optical" branches as well as low frequency acoustic branches at the long wave limit, as illustrated in Fig. 8. In that case, classical elasticity accounts for the long wave portions of only the acoustic branches. The appropriate extension [6] of classical elasticity to accommodate the long wave behavior of such polyatomic crystal is suggested by the fact that a lattice with a basis can be resolved into two or more interpenetrating Bravais lattices.

The simplest lattice with a basis is the Na-Cl type which has particles at the points (la, ma, na) of a simple-cubic lattice; but the particles at $l+m+n$ even have mass $\overset{1}{M}$, say, and those at $l+m+n$ odd have mass $\overset{2}{M}$, as represented in Fig. 9 by circles and dots, respectively. It may be seen that the lattice can be resolved into two, interpenetrating, face-centered, cubic lattices: one with particles of mass $\overset{1}{M}$ and the other with particles of mass $\overset{2}{M}$. The interactions between particles may be taken to be similar to those for the Gazis-Herman-Wallis lattice described in Article 2.i. The force constant between nearest neighbor (unlike) particles is designated by α. The force constants between next nearest neighbor (like) particles are assumed to be different: $\overset{1}{\beta}$ and $\overset{2}{\beta}$ for masses $\overset{1}{M}$ and $\overset{2}{M}$, respectively. The angular force constant, γ, is taken to be the same whether a particle of mass $\overset{1}{M}$ or $\overset{2}{M}$ is at the apex. Then Gazis and Wallis [25] find, for the particles at $l+m+n$ even, three equations of the type (2.1) with M and β replaced by $\overset{1}{M}$ and $\overset{1}{\beta}$; and, for the particles at $l+m+n$ odd, three equations of the type (2.1) with M and β replaced by $\overset{2}{M}$ and $\overset{2}{\beta}$. When the displacements

$$u_j^{\ell,m,n} = \overset{\nu}{A}_j\, e^{i(\ell\theta_1 + m\theta_2 + n\theta_3 - \omega t)} \tag{4.1}$$

with $\nu = 1$ and 2 for $\ell+m+n$ even and odd, respectively, are substituted in the six difference equations of motion, there results the dispersion relation

$$\begin{vmatrix} \overset{1}{d}_{11} & \overset{1}{d}_{12} & \overset{1}{d}_{13} & d_{11} & 0 & 0 \\ \overset{1}{d}_{21} & \overset{1}{d}_{22} & \overset{1}{d}_{23} & 0 & d_{22} & 0 \\ \overset{1}{d}_{31} & \overset{1}{d}_{32} & \overset{1}{d}_{33} & 0 & 0 & d_{33} \\ d_{11} & 0 & 0 & \overset{2}{d}_{11} & \overset{2}{d}_{12} & \overset{2}{d}_{13} \\ 0 & d_{22} & 0 & \overset{2}{d}_{21} & \overset{2}{d}_{22} & \overset{2}{d}_{23} \\ 0 & 0 & d_{33} & \overset{2}{d}_{31} & \overset{2}{d}_{32} & \overset{2}{d}_{33} \end{vmatrix} = 0, \tag{4.2}$$

where

$$\begin{aligned} \overset{\nu}{d}_{ij} &= \overset{\nu}{M}\omega^2 - 2(\alpha+8\gamma) - 4\overset{\nu}{\beta}\left(2 - \cos\theta_i \sum_{k\neq i}\cos\theta_k\right), \quad i=j, \\ \overset{\nu}{d}_{ij} &= -4(\overset{\nu}{\beta}+\gamma)\sin\theta_i \sin\theta_j, \quad i\neq j, \\ d_{ii} &= 2\alpha\cos\theta_i + 8\gamma\sum_{k\neq i}\cos\theta_k, \end{aligned} \tag{4.3}$$

in which i, j and k range over 1, 2, 3 and ν over 1, 2.

If we designate $\overset{1}{u}_i$ and $\overset{2}{u}_i$ as the displacements of particles with mass $\overset{1}{M}$ and $\overset{2}{M}$, respectively, and write

$$\overset{\nu}{u}_j^{\ell,m,n} = \overset{\nu}{A}_j\, e^{i(\ell\theta_1 + m\theta_2 + n\theta_3 - \omega t)} \tag{4.4}$$

for all ℓ, m, n, and adopt the notation (2.3) for finite difference operators, the same dispersion relation as (4.2) results from three equations of the type

$$\begin{aligned} \overset{1}{M}\overset{1}{u}_{1,tt}^{\ell,m,n} &= 2(\alpha+8\gamma)(\overset{2}{u}_1^{\ell,m,n} - \overset{1}{u}_1^{\ell,m,n}) + 2a^2\overset{1}{\beta}(2\Delta_1^2 + \Delta_2^2 + \Delta_3^2)\overset{1}{u}_1^{\ell,m,n} \\ &\quad + 4(\overset{1}{\beta}+\gamma)a^2(\Delta_1\Delta_2\overset{1}{u}_2^{\ell,m,n} + \Delta_1\Delta_3\overset{1}{u}_3^{\ell,m,n}) \\ &\quad + \overset{1}{\beta}a^4(\Delta_1^2\Delta_2^2 + \Delta_1^2\Delta_3^2)\overset{1}{u}_1^{\ell,m,n} \\ &\quad + \alpha a^2\Delta_1^2\overset{2}{u}_1^{\ell,m,n} + 4\gamma a^2(\Delta_2^2 + \Delta_3^2)\overset{2}{u}_1^{\ell,m,n} \end{aligned} \tag{4.5}$$

and three more obtained by interchange of superscripts 1 and 2. This form [6] is more convenient for passing to continuum limits since the

necessity for distinguishing between $\ell+m+n$ even and odd is dispensed with.

At long wave length and low frequency: $\overset{1}{u}_i = \overset{2}{u}_i = u_i$, say. Then employing the expansions (2.7), discarding derivatives higher than the second and adding corresponding members of the two sets of three equations of motion, we recover the equations of classical elasticity of the type (2.8) with

$$\rho = (\overset{1}{M}+\overset{2}{M})/2a^3 \tag{4.6}$$

and stiffness constants given by (2.6) with

$$\beta = (\overset{1}{\beta}+\overset{2}{\beta})/2. \tag{4.7}$$

At long wave lengths but not necessarily low frequency, (4.5) becomes, with $\overset{1}{M} = 2a^3\overset{1}{\rho}$,

$$\begin{aligned} a\overset{1}{\rho}\,\overset{1}{u}_{1,tt} &= a^{-2}(\alpha+8\gamma)(\overset{2}{u}_1-\overset{1}{u}_1) + \overset{1}{\beta}(2\partial_1^2+\partial_2^2+\partial_3^2)\overset{1}{u}_1 \\ &\quad + 2(\overset{1}{\beta}+\gamma)(\partial_1\partial_2\overset{1}{u}_2+\partial_1\partial_3\overset{1}{u}_3) \\ &\quad + \tfrac{1}{2}\alpha\,\partial_1^2\overset{2}{u}_1 + 2\gamma(\partial_1^2+\partial_2^2)\overset{2}{u}_1 . \end{aligned} \tag{4.8}$$

Thus, for the long wave approximation, there are three equations of the type (4.8) and three more obtained by interchange of superscripts 1 and 2. The six equations yield the long wave limits of the dispersion relation (4.2) for both the acoustic and optical branches.

A continuum theory that produces equations of the same form as (4.8) may be constructed as follows [6]. We consider two interpenetrating continua, identified by superscripts 1 and 2, representing the two face-centered cubic sub-lattices of the NaCl structure. The potential energy density is taken as a quadratic function of the strains of the two continua and their relative displacement and rotation. For the crystal class m3m, to which the face centered cubic and NaCl lattices belong, this is, with $\kappa=1,2$ and $\lambda=1,2$,

$$W = c_0^*(\overset{2}{S}_{ii}-\overset{1}{S}_{ii}) + \tfrac{1}{2}a^{**}u_i^*u_i^* + c^{**}\omega_{ij}^*\omega_{ij}^* + \tfrac{1}{2}\sum_{\kappa,\lambda} c_{ijk\ell}^{\kappa\lambda}\overset{\kappa}{S}_{ij}\overset{\lambda}{S}_{k\ell}, \tag{4.9}$$

where

$$u_i^* = (\overset{2}{u}_i - \overset{1}{u}_i), \quad \overset{\kappa}{s}_{ij} = \tfrac{1}{2}(\partial_i \overset{\kappa}{u}_j + \partial_j \overset{\kappa}{u}_i), \quad \omega_{ij}^* = \tfrac{1}{2}(\partial_i u_j^* - \partial_j u_i^*),$$
$$c_{ijkl}^{\kappa\lambda} = c_{ijkl}^{\lambda\kappa} = (c_{11}^{\kappa\lambda} - c_{12}^{\kappa\lambda} - 2c_{44}^{\kappa\lambda})\,\delta_{ijkl} + c_{12}^{\kappa\lambda}\,\delta_{ij}\delta_{kl} + c_{44}^{\kappa\lambda}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{4.10}$$

and the $\delta_{ij\ldots}$ are unity if all indices are alike and zero otherwise.

With kinetic energy density

$$T = \tfrac{1}{2}\sum_{\kappa} \overset{\kappa}{\rho}\, \overset{\kappa}{u}_{i,t}\, \overset{\kappa}{u}_{i,t} \tag{4.11}$$

and the potential energy density (4.9), Hamilton's variational principle, for independent variations $\delta\overset{1}{u}_i$ and $\delta\overset{2}{u}_i$, yields the six Euler equations

$$\begin{aligned} \overset{\kappa}{\rho}\,\overset{\kappa}{u}_{j,tt} = &-(-1)^{\kappa}\Big[a^{**}(\overset{2}{u}_j - \overset{1}{u}_j) + c^{**}\sum_{\lambda}\partial_i(\partial_i \overset{\lambda}{u}_j - \partial_j \overset{\lambda}{u}_i)\Big] \\ &+ \sum_{\lambda}\Big[(c_{11}^{\kappa\lambda} - c_{12}^{\kappa\lambda} - 2c_{44}^{\kappa\lambda})\,\delta_{ijkl}\,\partial_i\partial_k \overset{\lambda}{u}_l\Big] \\ &+ \sum_{\lambda}\Big[c_{12}^{\kappa\lambda}\,\partial_i\partial_j \overset{\lambda}{u}_i + c_{44}^{\kappa\lambda}\,\partial_i(\partial_i \overset{\lambda}{u}_j + \partial_j \overset{\lambda}{u}_i)\Big]. \end{aligned} \tag{4.12}$$

These become the six equations of the type (4.8) if we set

$$\begin{aligned} &ac_{11}^{\kappa\kappa} \quad 2ac_{44}^{\kappa\kappa} = 2\overset{\kappa}{\beta}, \qquad ac_{12}^{\kappa\kappa} = \beta + 2\gamma, \qquad c^{**} = 0, \\ &ac_{44}^{12} = -ac_{12}^{12} = 4\gamma, \qquad ac_{11}^{12} = \tfrac{1}{2}\alpha, \qquad a^{**} = (\alpha + 8\gamma)/a^3. \end{aligned} \tag{4.13}$$

Thus, the theory of a compound continuum, represented by the potential and kinetic energy densities (4.9) and (4.11), produces equations of motion which are the long wave limit of the Gazis-Wallis finite difference equations of an NaCl type lattice of mass particles.

It may be noted that the linear term in (4.9) is the energy density of a self-equilibrated initial stress which produces a surface energy of deformation analogous to that in the second strain gradient equations described in Article 3iii, but with the continuum representation of only nearest and next nearest neighbor interactions.

5. Molecular Crystals and Cosserat Continua

Crystals with identical groups of closely packed atoms, forming molecules, situated at the points of a lattice are termed molecular crystals if the intramolecular forces are large in comparison with the intermolecular forces [26]. In a monomolecular crystal, there is one molecule at each point of a Bravais lattice. The displacements of the mass centers of the molecules correspond to the displacements of the atoms of a monatomic lattice; and the associated equations of motion reduce to those of classical elasticity in the long wave approximation. However, the rotation and strain of the molecules themselves may also be taken into account. In the long wave approximation, these motions, which may be termed the micro-rotation and the micro-strain of a micro-structure (molecule), can be represented by an asymmetric tensor of the second rank, say ψ_{ij}. The antisymmetric part of the tensor:

$$\psi_{[ij]} = \frac{1}{2}\left(\psi_{ij} - \psi_{ji}\right) \tag{5.1}$$

describes the micro-rotation and the symmetric part:

$$\psi_{(ij)} = \frac{1}{2}\left(\psi_{ij} + \psi_{ji}\right) \tag{5.2}$$

describes the strain — both of which may be different from the rotation and strain calculated from the displacements of the mass centers.

The micro-rotation was taken into account in a continuum theory by E. and F. Cosserat [27] in 1909. Their equations were revived and applied to two-dimensional problems by Schaefer [28] in 1962. Subsequently, the Cosserat theory was termed "micropolar elasticity" by Eringen [29]. Comparisons of various forms of the theory and general solutions of the equations by Eringen [29], Aero and Kuvshinskii [30, 31], Neuber [32] and Mindlin [33] were given by Cowin [34,35] along with a more concise general solution. As is shown below, the Cosserat theory is the long wave approximation to a lattice theory

of monomolecular crystals. A direct correspondence between the Cosserat theory and the molecular crystal KNO_3 has recently been exhibited by Askar [36].

The long wave, low frequency limit of both the molecular lattice and Cosserat theories is the rotation gradient theory mentioned in Article 3i. This limiting form is the same as that obtained from the Cosserat theory by constraining the micro-rotation to be the same as the rotation calculated from the displacements. In fact, Toupin [37] refers to the rotation gradient theory as the "Cosserat theory with constrained rotations."

Extensions of the Cosserat theory to take into account the strain of the micro-structure were made in 1964 by Eringen [38] ("micromorphic" theory) Green and Rivlin [39] ("multipolar" theory) and Mindlin [40] ("micro structure" theory). In their simplest form, these theories are characterized by the potential energy density [40]

$$\begin{aligned} W = \tfrac{1}{2} c_{ijkl} S_{ij} S_{kl} + \tfrac{1}{2} b_{ijkl} \gamma_{ij} \gamma_{kl} + \tfrac{1}{2} a_{ijklmn} \kappa_{ijk} \kappa_{lmn} \\ + d_{ijklm} \gamma_{ij} \kappa_{klm} + f_{ijklm} \kappa_{ijk} S_{lm} + g_{ijkl} \gamma_{ij} S_{kl} , \end{aligned} \tag{5.3}$$

where S_{ij} is the ordinary strain (macro-strain):

$$S_{ij} = \tfrac{1}{2}(\partial_i u_j + \partial_j u_i), \tag{5.4}$$

γ_{ij} is the relative deformation (the difference between the displacement gradient and the micro-deformation):

$$\gamma_{ij} = \partial_i u_j - \psi_{ij} \tag{5.5}$$

and κ_{ijk} is the gradient of the micro-deformation:

$$\kappa_{ijk} = \partial_i \psi_{jk} . \tag{5.6}$$

In the centrosymmetric, isotropic case [40], d_{ijklm} and f_{ijklm}, in (5.3), are zero and

$$c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}),$$

$$
\begin{aligned}
g_{ijkl} &= g_1\delta_{ij}\delta_{kl} + g_2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \\
b_{ijkl} &= b_1\delta_{ij}\delta_{kl} + b_2\delta_{ik}\delta_{jl} + b_3\delta_{il}\delta_{jk}, \\
a_{ijklmn} &= a_1(\delta_{ij}\delta_{kl}\delta_{mn} + \delta_{jk}\delta_{in}\delta_{lm}) + a_2(\delta_{ij}\delta_{km}\delta_{nl} + \delta_{ki}\delta_{jn}\delta_{lm}) \\
&\quad + a_3\delta_{ij}\delta_{kn}\delta_{lm} + a_4\delta_{jk}\delta_{il}\delta_{mn} + a_5(\delta_{jk}\delta_{im}\delta_{nl} + \delta_{ki}\delta_{jl}\delta_{mn}) \\
&\quad + a_8\delta_{ki}\delta_{jm}\delta_{nl} + a_{10}\delta_{il}\delta_{jm}\delta_{kn} + a_{11}(\delta_{jl}\delta_{km}\delta_{in} + \delta_{kl}\delta_{im}\delta_{jn}) \\
&\quad + a_{13}\delta_{il}\delta_{jn}\delta_{km} + a_{14}\delta_{jl}\delta_{kn}\delta_{im} + a_{15}\delta_{kl}\delta_{in}\delta_{jm}.
\end{aligned}
\tag{5.7}
$$

The associated kinetic energy density is

$$
T = \tfrac{1}{2}\rho\dot{u}_j\dot{u}_j + \tfrac{1}{6}\rho d^2\dot{\psi}_{ij}\dot{\psi}_{ij}, \tag{5.8}
$$

where ρ is the mass density and d is a characteristic length dimension of the molecule (half the edge length in the case of cubic).

The complete set of dispersion relations for plane waves in such a material with a deformable microstructure is given in [40] and exhibits twelve branches: the usual three acoustic branches and, in addition, nine optical branches, i.e. branches with non zero frequency at infinite wave length. At low frequencies and long wave lengths, the differential equations of motion and the dispersion relations reduce to those of the first strain gradient theory.

In molecular crystals, the most interesting of the optical branches is the relatively low frequency "librational" or "soft optical" branch (labelled TRO, for transverse rotational optical in [40]) that is coupled to a transverse acoustic branch. The equations of motion for this pair of coupled modes are obtained by setting $\psi_{(12)} = 0$ (thereby eliminating the shear micro strain) in the first and third of Eqs. (8.5) in [40], with the result

$$
\begin{aligned}
\bar{k}_{11}\partial_1^2 u_2 - \bar{k}_{13}\partial_1\psi_{[12]} &= \rho\ddot{u}_2, \\
\bar{k}_{13}\partial_1 u_2 + \bar{k}_{33}\partial_1^2\psi_{[12]} - 2\bar{k}_{13}\psi_{[12]} &= \tfrac{2}{3}\rho d^2\ddot{\psi}_{[12]},
\end{aligned}
\tag{5.9}
$$

where

$$
\begin{aligned}
\bar{k}_{11} &= \mu + 2g_2 + b_2, \quad \bar{k}_{13} = b_2 - b_3, \\
\bar{k}_{33} &= -2a_2 + a_3 + a_8 + 2a_{10} - 2a_{13} + a_{14} + a_{15}.
\end{aligned}
\tag{5.10}
$$

Since $\psi_{(ij)} = 0$ in (5.9), they are equations of a Cosserat continuum. Setting

$$u_2 = A e^{i(\xi x_1 - \omega t)}, \qquad \psi_{[12]} = B e^{i(\xi x_1 - \omega t)} \tag{5.11}$$

and eliminating A and B, we obtain the dispersion relation

$$\begin{vmatrix} \bar{k}_{11}\xi^2 - \rho\omega^2 & \bar{k}_{13}\xi \\ \bar{k}_{13}\xi & \bar{k}_{33}\xi^2 + 2\bar{k}_{13} - \frac{2}{3}\rho d^2\omega^2 \end{vmatrix} = 0. \tag{5.12}$$

The two branches of (5.12) have ordinates and slopes at $\xi = 0$ as follows:

$$\begin{aligned} &\text{acoustic branch:} \quad \omega\Big]_{\xi=0} = 0, \quad \frac{d\omega}{d\xi}\Big]_{\xi=0} = \left(\frac{2\bar{k}_{11} - \bar{k}_{13}}{2\rho}\right)^{1/2}; \\ &\text{soft optical branch:} \quad \omega\Big]_{\xi=0} = \left(\frac{3\bar{k}_{13}}{\rho d^2}\right)^{1/2}, \quad \frac{d\omega}{d\xi}\Big]_{\xi=0} = 0. \end{aligned} \tag{5.13}$$

It may be verified that (5.9) are the long wave limits of the finite difference equations of motion of a linear lattice of dumbell molecules [2, Article 10]. We consider a line of molecules of length $2d$, spacing a, mass m and moment of inertia I with transverse displacement u_n and rotation ψ_n at lattice point n, as illustrated in Fig. 10. The potential energy of the lattice may be taken as

$$\begin{aligned} \varphi = a^{-2} \Sigma \big[&\tfrac{1}{2}\alpha_1 (u_{n+1} - u_n)^2 + \tfrac{1}{2}\alpha_2 (u_{n+1} - u_n - d\psi_n)^2 \\ &+ \tfrac{1}{2}\alpha_3 d^2 (\psi_{n+1} - \psi_n)^2 + \alpha_4 (u_{n+1} - u_n)(u_{n+1} - u_n - d\psi_n) \big] \end{aligned} \tag{5.14}$$

where $\alpha_1, \ldots \alpha_4$ are force constants. Comparing with (5.3), we see that (5.14) is the one-dimensional, finite difference analogue for the centrosymmetric case, i.e.

$$\begin{gathered} d_{ijklm} = 0, \quad f_{ijklm} = 0 \\ s_{ij} = \tfrac{1}{2}(\partial_i u_j + \partial_j u_i) \to (u_{n+1} - u_n)/a, \quad \gamma_{ij} = \partial_i u_j - \psi_{ij} \to (u_{n+1} - u_n - d\psi_n)/a, \\ \kappa_{ijk} = \partial_i \psi_{jk} \to (\psi_{n+1} - \psi_n)/a. \end{gathered} \tag{5.15}$$

With finite difference operators Δ^+, Δ° and Δ^2 again defined as in (2.3), the equations of motion are given by

$$-\frac{\partial\varphi}{\partial u_n} = (\alpha_1+\alpha_2+2\alpha_4)\,\Delta^2 u_n - \frac{d}{a}(\alpha_2+\alpha_4)\Delta^- \psi_n = m\ddot{u}_n a^{-2}$$

$$-\frac{\partial\varphi}{\partial\psi_n} = \frac{d}{a}(\alpha_2+\alpha_4)\Delta^+ u_n + \alpha_3 d^2\Delta^2\psi_n - \frac{d^2}{a^2}\alpha_2\psi_n = I\ddot{\psi}_n a^{-2} \qquad (5.16)$$

Insert

$$u_n = Ae^{i(\xi na-\omega t)}, \quad \psi_n = Be^{i(\xi na-\omega t)} \qquad (5.17)$$

in (5.16) and find the dispersion relation

$$\begin{vmatrix} 2(\alpha_1+\alpha_2+2\alpha_4)(\cos\xi a-1) - m\omega^2 & d(\alpha_2+\alpha_4)(\cos\xi a - 1 - \sin\xi a) \\ d(\alpha_2+\alpha_4)(\cos\xi a - 1 + \sin\xi a) & 2\alpha_3 d^2(\cos\xi a-1) - \alpha_2 d^2 + I\omega^2 \end{vmatrix} = 0 \qquad (5.18)$$

which is illustrated in Fig. 11. The ordinates and slopes of the two branches at $\xi = 0$ are:

$$\text{acoustic branch:}\quad \omega\Big]_{\xi=0} = 0, \quad \frac{d\omega}{d\xi}\Big]_{\xi=0} = \left[\frac{\alpha_2(\alpha_1+2\alpha_2)+\alpha_4(4\alpha_2+\alpha_4)}{m\alpha_2 a^{-2}}\right]^{1/2}$$

$$\text{soft optical branch:}\quad \omega\Big]_{\xi=0} = d\sqrt{\frac{\alpha_2}{I}}, \quad \frac{d\omega}{d\xi}\Big]_{\xi=0} = 0. \qquad (5.19)$$

If, in the finite difference equations of motion (5.16), we set

$$a\bar{k}_{11} = \alpha_1+\alpha_2+2\alpha_4, \quad a\bar{k}_{13} = (\alpha_2+\alpha_4)d/a = \alpha_2 d^2/2a^2, \quad a\bar{k}_{33} = \alpha_3 d^2,$$
$$a^3\rho \to m, \quad I \to \tfrac{2}{3}\rho d^2 a^3 \qquad (5.20)$$

and retain only the first term in the expansion of each of the difference operators in series of differential operators, we find that (5.16) reduce to the differential equations of motion (5.9) of the Cosserat continuum. Similarly, if we insert (5.20) in the expressions (5.19) for the long wave limits of the two branches of the lattice dispersion relation, we find the corresponding expressions (5.13) for the Cosserat continuum.

An alternative formulation of the lattice equations and an application to KNO_3 are given by Askar [ ].

6. Classical Piezoelectricity

The classical, linear theory of elastic dielectrics (piezoelectricity) is expressed in terms of twenty-five variables [3, 41]:

u_i Mechanical displacement
S_{ij} Strain
T_{ij} Stress
E_i Electric field
D_i Electric displacement
P_i Polarization
φ Electric potential

These variables are linked by twenty-five equations:
(a) stress-equations of motion

$$T_{ij,i} + f_j = \rho \ddot{u}_j \; ; \tag{6.1}$$

(b) equations of the electrostatic field

$$D_{i,i} = 0 \; , \tag{6.2}$$

$$E_i = -\varphi_{,i} \; ; \tag{6.3}$$

(c) strain-displacement relations

$$S_{ij} = \tfrac{1}{2}(u_{j,i} + u_{i,j}) \tag{6.4}$$

(d) constitutive relations

$$T_{ij} = c^E_{ijkl} S_{kl} - e_{kij} E_k \, , \tag{6.5}$$

$$D_j = e_{jkl} S_{kl} + \epsilon^S_{jk} E_k \, , \tag{6.6}$$

$$P_i = D_i - \epsilon_0 E_i \; , \tag{6.7}$$

where

c^{E}_{ijkl} = elastic stiffness (E_i = constant)

e_{ijk} = piezoelectric stress-constant

ϵ^{S}_{ij} = permittivity (S_{ij} = constant)

ϵ_0 = permittivity of a vacuum

The equations of motion may be reduced to four by elimination of all the variables except u_i and φ:

$$c^{E}_{ijkl} u_{k,li} + e_{kij} \varphi_{,ki} + f_j = \rho \ddot{u}_j , \tag{6.8}$$

$$e_{kij} u_{i,jk} - \epsilon^{S}_{ij} \varphi_{,ij} = 0. \tag{6.9}$$

A linear version of a variational principle due to Toupin [42] may be employed to produce equivalent equations of equilibrium, as follows.

First, separate the energy density, W, of the dielectric into the stored energy of deformation and polarization, $\bar{W}^L$, and a remainder which is the energy density of the Maxwell electric self-field:

$$\bar{W} = W^L(S_{ij}, P_i) + \tfrac{1}{2}\epsilon_0 \varphi_{,i}\varphi_{,i} . \tag{6.10}$$

Then define an electric enthalpy [41]

$$H = \bar{W} - E_i D_i . \tag{6.11}$$

Upon substituting (6.10), (6.7) and (6.5) in (6.11) we find

$$H = W^L(S_{ij}, P_i) - \tfrac{1}{2}\epsilon_0 \varphi_{,i}\varphi_{,i} + \varphi_{,i} P_i . \tag{6.12}$$

Consider a body occupying a volume V bounded by a surface S separating V from an outer vacuum V'. For such a system, the version of Toupin's principle that leads to equations equivalent to those preceding, for the case of equilibrium, is

$$-\delta\int_{V^*} H\, dV + \int_V (f_i \delta u_i + E^{o}_i \delta P_i)\, dV + \int_S t_i \delta u_i\, dS = 0, \tag{6.13}$$

for independent variations of u_i, P_i and φ. In (6.13), $V^* = V + V'$ and t_i is the surface traction across S and E_i° is the external electric field. Now,

$$\delta H = \frac{\partial W^L}{\partial S_{ij}}\,\delta S_{ij} + \frac{\partial W^L}{\partial P_i}\,\delta P_i - \epsilon_0\,\varphi_{,i}\,\delta\varphi_{,i} + \varphi_{,i}\,\delta P_i + P_i\,\delta\varphi_{,i}\,. \tag{6.14}$$

Define a stress T_{ij} and an effective local electric force E_i^L by

$$T_{ij} = \frac{\partial W^L}{\partial S_{ij}}\,, \qquad E_i^L = -\frac{\partial W^L}{\partial P_i}\,. \tag{6.15}$$

Note that, since $T_{ij} = T_{ji}$ and

$$S_{ij} = \tfrac{1}{2}\left(u_{j,i} + u_{i,j}\right), \tag{6.16}$$

$$\begin{aligned} T_{ij}\,\delta S_{ij} &= T_{ij}\,\delta u_{j,i} = \left(T_{ij}\,\delta u_j\right)_{,i} - T_{ij,i}\,\delta u_j\,,\\ \varphi_{,i}\,\delta\varphi_{,i} &= \left(\varphi_{,i}\,\delta\varphi\right)_{,i} - \varphi_{,ii}\,\delta\varphi\,,\\ P_i\,\delta\varphi_{,i} &= \left(P_i\,\delta\varphi\right)_{,i} - P_{i,i}\,\delta\varphi\,, \end{aligned}$$

by the chain rule of differentiation. Then

$$\delta H = -T_{ij,i}\,\delta u_j - \left(E_i^L - \varphi_{,i}\right)\delta P_i - \left(-\epsilon_0\varphi_{,ii} + P_{i,i}\right)\delta\varphi + \left[T_{ij}\,\delta u_j + \left(-\epsilon_0\varphi_{,i} + P_i\right)\delta\varphi\right]_{,i}\,. \tag{6.17}$$

Noting that $V^* = V + V'$ and that u_i and P_i do not exist in V', we find, after applying the divergence theorem,

$$\begin{aligned} -\delta\int_V H\,dV = &\int_V \left[T_{ij,i}\,\delta u_j + \left(E_i^L - \varphi_{,i}\right)\delta P_i + \left(-\epsilon_0\varphi_{,ii} + P_{i,i}\right)\delta\varphi\right]dV\\ &- \int_S n_i\left[T_{ij}\,\delta u_j + \left(-\epsilon_0\varphi_{,i} + P_i\right)\delta\varphi\right]dS\,, \end{aligned} \tag{6.18a}$$

$$-\delta\int_{V'} H\,dV = -\int_{V'} \epsilon_0\,\varphi_{,ii}\,\delta\varphi\,dV - \int_S \epsilon_0\,n_i\,\varphi_{,i}\,\delta\varphi\,dS\,. \tag{6.18b}$$

Hence, (6.13) becomes

$$\begin{aligned} &\int_V \left[\left(T_{ij,i} + f_j\right)\delta u_j + \left(E_i^L - \varphi_{,i} + E_i^\circ\right)\delta P_i + \left(-\epsilon_0\varphi_{,ii} + P_{i,i}\right)\delta\varphi\right]dV - \int_{V'} \epsilon_0\,\varphi_{,ii}\,\delta\varphi\,dV\\ &+ \int_S \left[\left(t_j - n_i T_{ij}\right)\delta u_j + n_i\left(\epsilon_0 [\![\varphi_{,i}]\!] - P_i\right)\delta\varphi\right]dS = 0\,, \end{aligned} \tag{6.19}$$

where $[\![\varphi_{,i}]\!]$ is the jump in $\varphi_{,i}$ across S. Then the Euler equations

$$\left.\begin{aligned} T_{ij,i} + f_j &= 0, \\ E_i^L - \varphi_{,i} + E_i^o &= 0, \\ -\epsilon_0 \varphi_{,ii} + P_{i,i} &= 0, \end{aligned}\right\} \text{ in } V, \tag{6.20}$$

$$\varphi_{,ii} = 0 \quad \text{in } V' \tag{6.21}$$

and the natural boundary conditions

$$\left.\begin{aligned} n_i T_{ij} &= t_j \\ n_i(-\epsilon_0 [\![\varphi_{,i}]\!] + P_i) &= 0, \end{aligned}\right\} \text{ on } S, \tag{6.22}$$

follow from (6.19). In (6.22), $n_i(-\epsilon_0 [\![\varphi_{,i}]\!] + P_i)$ is the surface charge.

The energy density of deformation and polarization is taken to be

$$W^L = \tfrac{1}{2} a^s_{ij} P_i P_j + \tfrac{1}{2} c^P_{ijkl} S_{ij} S_{kl} + f_{klj} S_{ij} P_k \tag{6.23}$$

so that, from (6.15),

$$\begin{aligned} -E_j^L &= a^s_{jk} P_k + f_{jkl} S_{kl}, \\ T_{ij} &= f_{kij} P_k + c^P_{ijkl} S_{kl}. \end{aligned} \tag{6.24}$$

Equations (6.16), (6.20), (6.21) and (6.24), with boundary conditions (6.22), constitute a linear version of the equations of equilibrium of elastic dielectrics in the form given by Toupin [42].

The relations between the new constants a^s_{ij}, f_{ijk} and c^P_{ijkl} and the IRE Standard [43] ones are found as follows.

From (6.3) and the second of (6.20) (omitting E_i^o as in the usual formulation) $E_i^L = -E_i$. Hence, the first of (6.24) becomes

$$E_j = a^s_{jk} P_k + f_{jkl} S_{kl}. \tag{6.25}$$

Now the ratio of P to $\epsilon_0 E$ is the dielectric susceptibility. Hence a^s_{ij} is proportional to the reciprocal susceptibility at constant strain (χ^S_{ij}):

$$a^s_{ij} = \epsilon_0^{-1} \chi^S_{ij}. \tag{6.26}$$

With (6.26), (6.25) becomes

$$E_j = \epsilon_0^{-1}\chi_{jk}P_k + f_{jk\ell}S_{k\ell}. \tag{6.27}$$

Define susceptibility at constant strain, η^S_{ij}, according to

$$\eta^S_{ij}\chi^S_{jk} = \delta_{ij} \tag{6.28}$$

and multiply both sides of (6.27) by $\epsilon_0\eta_{mj}$ to get

$$\epsilon_0\eta^S_{mj}E_j = P_m + \epsilon_0\eta^S_{mj}f_{jk\ell}S_{k\ell}. \tag{6.29}$$

Then eliminate P between (6.29) and (6.1), with the result

$$D_i = -\epsilon_0\eta^S_{ij}f_{jk\ell}S_{k\ell} + \epsilon_0(\delta_{ij} + \eta^S_{ij})E_j. \tag{6.30}$$

Accordingly, comparing (6.30) with (6.6), we find

$$e_{jk\ell} = -\epsilon_0\eta^S_{ij}f_{ik\ell}, \qquad \text{or} \qquad f_{jk\ell} = -\epsilon_0^{-1}\chi^S_{ij}e_{ik\ell}; \tag{6.31}$$

$$\epsilon^S_{ij} = \epsilon_0(\delta_{ij} + \eta^S_{ij}), \qquad \text{or} \qquad \eta^S_{ij} = \epsilon_0^{-1}\epsilon^S_{ij} - \delta_{ij}. \tag{6.32}$$

To find $c^P_{ijk\ell}$ in terms of $c^E_{ijk\ell}$, first substitute the expression for P_i, given in terms of E_i and S_{ij} in (6.29), into the second of (6.24):

$$T_{ij} = f_{mij}(\epsilon_0\eta^S_{mk}E_k - \epsilon_0\eta^S_{mn}f_{nk\ell}S_{k\ell}) + c^P_{ijk\ell}S_{k\ell}$$

or, from (6.31),

$$T_{ij} = (c^P_{ijk\ell} - \epsilon_0\eta^S_{mn}f_{mij}f_{nk\ell})S_{k\ell} - e_{kij}E_k. \tag{6.33}$$

Comparing (6.33) with (6.5), we see that

$$c^E_{ijk\ell} = c^P_{ijk\ell} - \epsilon_0\eta^S_{mn}f_{mij}f_{nk\ell} \tag{6.34}$$

or, from (6.31),

$$c^P_{ijk\ell} = c^E_{ijk\ell} + \epsilon_0^{-1}\chi^S_{mn}e_{mij}e_{nk\ell}. \tag{6.35}$$

With the aid of the foregoing expressions for the constants a^S_{ij},

c^D_{ijkl} and f_{ijk}, we may reduce the equations of equilibrium (6.20) and the constitutive equations (6.24) to the classical form of equations on u_i and φ, given in (6.8) and (6.9), by elimination of P_i. First, to solve the first of (6.24) for P_i, recall that the reciprocal of α^S_{ij} is $\epsilon_0 \eta^S_{ij}$. Then, upon multiplication, we have

$$P_i = -\epsilon_0 \eta^S_{ij}(E^L_j + f_{jkl} S_{kl}). \tag{6.36}$$

Substitute this for P_i in the second of (6.24) to obtain

$$T_{ij} = -f_{kij}\,\epsilon_0 \eta^S_{km}(E^L_m + f_{mpq} S_{pq}) + c^P_{ijkl} S_{kl}.$$

From the second equilibrium equation, $E^L_i = \varphi_{,i}$, again omitting L^0_i. Also, $S_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j})$. Hence

$$T_{ij,i} = (c^P_{ijkl} - \epsilon_0 \eta^S_{mn} f_{mij} f_{nkl}) u_{k,li} - \epsilon_0 \eta^S_{km} f_{kij}\, \varphi_{,mi}$$

Then, from the first of (6.31) and from (6.34),

$$T_{ij,i} + f_j = c^E_{ijkl} u_{k,li} + e_{kij}\, \varphi_{,ki} + f_j$$

which is the left hand side of (6.8), as required.

Next, from (6.36),

$$\begin{aligned} P_{i,i} &= -\epsilon_0 \eta^S_{ij}(E^L_{j,i} + f_{jkl} S_{kl,i}) \\ &= -\epsilon_0 \eta^S_{ij}\, \varphi_{,ij} - \epsilon_0 \eta^S_{ij} f_{jkl} u_{k,li}. \end{aligned}$$

Hence, the left hand side of the last of the equilibrium equations (6.20) becomes

$$-\epsilon_0 \varphi_{,ii} + P_{i,i} = -\epsilon_0 \eta^S_{ij} f_{jkl} u_{k,li} - \epsilon_0(\delta_{ij} + \eta^S_{ij})\varphi_{,ij}$$

or, from the first of (6.31) and (6.32),

$$-\epsilon_0 \varphi_{,ii} + P_{i,i} = e_{ikl} u_{k,li} - \epsilon^S_{ij} \varphi_{,ij}$$

which is the left hand side of (6.9), as required.

7. Polarization Gradient

Toupin's form of the classical equations of elastic dielectrics reveals an omission in the classical theory. His equation

$$E_i^L - \varphi_{,i} + E_i^0 = 0$$

is the "equation of intramolecular force balance" [42] which he derives from fundamental considerations of the equilibrium of electrical forces, but which does not appear in the usual formulations. Granted the validity of the equation, it is significant that no boundary condition is associated with it. Whereas there is an equilibrium equation associated with each of the variables u_i, φ and P_i, only u_i and φ are accompanied by boundary conditions. There is no coefficient of δP_i in the surface integral in (6.10) to complement that in the volume integral. This lack can be traced back to the absence of a functional dependence of W^L on the polarization gradient $P_{j,i}$. In fact, if we were to start by assuming dependence of W^L on the displacement and polarization and their gradients and truncate after the first gradient, $P_{j,i}$ would remain along with S_{ij} and P_i. Only u_i and the antisymmetric part of $u_{j,i}$ would have to be discarded -- on the grounds of required translational and rotational invariance of W^L. The only justification for discarding $P_{j,i}$ would be its possible lack of importance judged on practical considerations. However, as will be shown, $P_{j,i}$ supplies terms found in the long wave limits of finite difference equations of lattice theories of crystals and also extends the continuum theory to accommodate observed physical phenomena.

To extend Toupin's variational principle to account for the contribution of the polarization gradient, it is only necessary to replace (6.12) with

$$H = W^L(S_{ij}, P_i, P_{j,i}) - \tfrac{1}{2}\epsilon_0 \varphi_{,i}\varphi_{,i} + \varphi_{,i}P_i . \tag{7.1}$$

In addition, we shall include the kinetic energy so that (6.13) becomes

$$\delta\int_{t_0}^{t_1}dt\int_{V^*}(\tfrac{1}{2}\rho\dot{u}_i\dot{u}_i-H)dV+\int_{t_0}^{t_1}dt\left[\int_V(f_i\delta u_i+E_i^0\delta P_i)dV+\int_S t_i\delta u_i dS\right]=0, \tag{7.2}$$

for independent variations of u_i, φ and P_i between fixed limits at times t_0 and t_1.

The only additional equations involved are a new definition,

$$E_{ij}=\frac{\partial W^L}{\partial P_{j,i}}, \tag{7.3}$$

and two integrations:

$$\tfrac{1}{2}\delta\int_{t_0}^{t_1}\dot{u}_i\dot{u}_i dt=\int_{t_0}^{t_1}\dot{u}_i\delta\dot{u}_i dt=\dot{u}_i\delta u_i\Big]_{t_0}^{t_1}-\int_{t_0}^{t_1}\ddot{u}_i\delta u_i dt=-\int_{t_0}^{t_1}\ddot{u}_i\delta u_i dt,$$

$$\int_V E_{ij}\delta P_{j,i}dV=\int_V[(E_{ij}\delta P_j)_{,i}-E_{ij,i}\delta P_j]dV=\int_S n_iE_{ij}\delta P_j dS-\int_V E_{ij,i}\delta P_j dV.$$

With these results and (6.18), (7.2) becomes

$$\int_{t_0}^{t_1}dt\int_V[(T_{ij,i}+f_j-\rho\ddot{u}_j)\delta u_j+(E_{ij,i}+E_j^L-\varphi_{,j}+E_j^0)\delta P_j+(-\epsilon_0\varphi_{,ii}+P_{i,i})\delta\varphi]dV$$

$$-\int_{t_0}^{t_1}dt\int_{V'}\epsilon_0\varphi_{,ii}\delta\varphi dV+\int_{t_0}^{t_1}dt\int_S[(t_j-n_iT_{ij})\delta u_j-n_iE_{ij}\delta P_j+n_i(\epsilon_0[\![\varphi_{,i}]\!]-P_i)\delta\varphi]dS=0. \tag{7.4}$$

Then the Euler equations are

$$\left.\begin{aligned}T_{ij,i}+f_j&=\rho\ddot{u}_j,\\ E_{ij,i}+E_j^L-\varphi_{,j}+E_j^0&=0,\\ -\epsilon_0\varphi_{,ii}+P_{i,i}&=0;\end{aligned}\right\}\text{ in }V \tag{7.5}$$

$$\varphi_{,ii}=0\text{ in }V', \tag{7.6}$$

with natural boundary conditions

$$\begin{aligned}n_iT_{ij}&=t_j,\\ n_iE_{ij}&=0,\\ n_i(-\epsilon_0[\![\varphi_{,i}]\!]+P_i)&=0.\end{aligned} \tag{7.7}$$

For W^L, we take

$$W^L=b_{ij}^0P_{j,i}+\tfrac{1}{2}a_{ij}^{SG}P_iP_j+\tfrac{1}{2}b_{ijkl}^{PS}P_{j,i}P_{l,k}+\tfrac{1}{2}c_{ijkl}^{PG}S_{ij}S_{kl}$$
$$+d_{ijkl}^{P}P_{j,i}S_{kl}+f_{ijk}^{G}P_iS_{jk}+j_{ijk}^{S}P_iP_{k,j}. \tag{7.8}$$

The superscripts S, P, G, designating fixed strain, polarization and polarization gradient, respectively, will be omitted in the sequel where no ambiguity results.

Substituting (7.8) in (6.15) and (7.3), we find

$$
\begin{aligned}
-E_j^L &= a_{jk} P_k + j_{jkl} P_{l,k} + f_{jkl} S_{kl}, \\
E_{ij} &= j_{kij} P_k + b_{ijkl} P_{l,k} + d_{ijkl} S_{kl} + b_{ij}^{0}, \\
T_{ij} &= f_{kij} P_k + d_{klij} P_{l,k} + c_{ijkl} S_{kl}.
\end{aligned}
\tag{7.9}
$$

The field equations (7.5) and (7.6), the constitutive equations (7.9) and the strain-displacement relation $S_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j})$ comprise the equations of the augmented theory [44]. It is apparent, from the form of the integrand of the surface integral in (1.4), what boundary conditions other than (1.1) are admissible. Thus, in place of the traction $n_i T_{ij}$, may be substituted the displacement u_i or a component of either and the resultant of the other in the plane at right angles. The same possibilities are open for $n_i E_{ij}$ and P_i. Finally, either the surface charge $n_i(-\epsilon_0 [\![\varphi_{,i}]\!] + P_i)$ or the potential φ may be specified. Of prime importance is the fact that <u>both</u> the potential φ and the polarization P_i may be specified. This is a latitude not permissible in the classical theory.

One of the novel properties of the augmented theory of elastic dielectrics is its accommodation of an electromechanical interaction even for materials with centrosymmetric physical properties. This may be seen by inspection of the energy density W^L as given in (7.8). For centrosymmetry, $f_{ijk} = j_{ijk} = 0$, since there are no centrosymmetric tensors of odd rank. However, this still leaves d_{ijkl} which is the coefficient of an electromechanical coupling term in the augmented theory, but does not appear in the classical theory.

As an example of crystallographic centrosymmetry, consider the cubic point group m3m (International), O_h (Schoenflies), the generators for which are [45]

$$
\begin{Vmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{Vmatrix}
\begin{Vmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{Vmatrix}
\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{Vmatrix}
\tag{7.10}
$$

Applying these to the coefficients in (7.8), we find

$$
\begin{aligned}
&f_{ijk} = 0, \quad j_{ijk} = 0, \\
&a_{ij} = a_{11}\delta_{ij}, \quad \overset{\circ}{b}_{ij} = b_0\delta_{ij}, \\
&b_{ijkl} = b\,\delta_{ijkl} + b_{12}\delta_{ij}\delta_{kl} + b_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + b_{77}(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}), \\
&c_{ijkl} = c\,\delta_{ijkl} + c_{12}\delta_{ij}\delta_{kl} + c_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \\
&d_{ijkl} = d\,\delta_{ijkl} + d_{12}\delta_{ij}\delta_{kl} + d_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),
\end{aligned}
\tag{7.11}
$$

where

$$
b = b_{11} - b_{12} - 2b_{44}, \quad c = c_{11} - c_{12} - 2c_{44}, \quad d = d_{11} - d_{12} - 2c_{44}. \tag{7.12}
$$

Insertion of (7.11) in the constitutive equations (7.9) reduces the latter to

$$
\begin{aligned}
-E_i^L &= a_{11}P_i, \\
E_{ij} &= b\,\delta_{ijkl}P_{l,k} + b_{12}\delta_{ij}P_{k,k} + b_{44}(P_{j,i} + P_{i,j}) + b_{77}(P_{j,i} - P_{i,j}) + b_0\delta_{ij} \\
&\quad + d\,\delta_{ijkl}S_{kl} + d_{12}\delta_{ij}S_{kk} + 2d_{44}S_{ij}, \\
T_{ij} &= d\,\delta_{ijkl}P_{l,k} + d_{12}\delta_{ij}P_{k,k} + d_{44}(P_{j,i} + P_{i,j}) + c\,\delta_{ijkl}S_{kl} + c_{12}\delta_{ij}S_{kk} + 2c_{44}S_{ij}.
\end{aligned}
\tag{7.13}
$$

The equations of motion on u_i, P_i and φ are obtained by substituting (7.13) in (7.5) and employing the strain-displacement relation, with the result:

$$
\begin{aligned}
&c\delta_{ijkl}u_{l,ki} + c_{12}u_{k,kj} + c_{44}(u_{j,ii} + u_{i,ji}) + d\,\delta_{ijkl}P_{l,ki} + d_{12}P_{k,kj} + d_{44}(P_{j,ii} + P_{i,ji}) + f_j = \rho\ddot{u}_j, \\
&d\,\delta_{ijkl}u_{l,ki} + d_{12}u_{k,kj} + d_{44}(u_{j,ii} + u_{i,ji}) + b\,\delta_{ijkl}P_{l,ki} + b_{12}P_{k,kj} + b_{44}(P_{j,ii} + P_{i,ji}) \\
&\qquad + b_{77}(P_{j,ii} - P_{i,ji}) - a_{11}P_j - \varphi_{,j} + E_j^{\circ} = 0, \\
&\qquad -\epsilon_0\varphi_{,ii} + P_{i,i} = 0.
\end{aligned}
\tag{7.14}
$$

In the one dimensional case,

$$
u_1 = u_1(x_1, t), \quad u_2 = u_3 = 0, \quad P_1 = P_1(x_1, t), \; P_2 = P_3 = 0, \quad \varphi = \varphi(x_1, t), \tag{7.15}
$$

and in the absence of extrinsic fields f_i and E_i°, (7.14) reduce to

$$
\begin{aligned}
&c_{11}\partial_1^2 u_1 + d_{11}\partial_1^2 P_1 = \rho\ddot{u}_1, \\
&d_{11}\partial_1^2 u_1 + b_{11}\partial_1^2 P_1 - a_{11}P_1 - \partial_1\varphi = 0, \\
&-\epsilon_0\partial_1^2\varphi + \partial_1 P_1 = 0.
\end{aligned}
\tag{7.16}
$$

To obtain the dispersion relation for (7.16), let

$$u_1 = Ae^{i(\xi x_1 - \omega t)}, \quad P_1 = Be^{i(\xi x_1 - \omega t)}, \quad \varphi = Ce^{i(\xi x_1 - \omega t)}. \tag{7.17}$$

Upon substituting (7.17) into (7.16) and eliminating A, B and C, we obtain

$$\begin{vmatrix} c_{11}\xi^2 - \rho\omega^2 & d_{11}\xi^2 \\ d_{11}\xi^2 & b_{11}\xi^2 + a_{11} + \epsilon_0^{-1} \end{vmatrix} = 0. \tag{7.18}$$

This is a quadratic equation in ξ^2, so that there are two branches. Positive definiteness of the energy density requires

$$a_{11} > 0, \quad b_{11}c_{11} - d_{11}^2 > 0. \tag{7.19}$$

Consequently one of the roots ξ^2 is positive real and the other is negative real. Thus, one of the branches of the dispersion relation is real and the other is imaginary. The behavior of the real branch at low frequency is given by

$$\lim_{\substack{\omega \to 0 \\ \xi \to 0}} \frac{\omega}{\xi} = \sqrt{\frac{c_{11}}{\rho}}. \tag{7.20}$$

The limit of the imaginary branch at zero frequency is

$$\lim_{\substack{\omega \to 0 \\ \xi \neq 0}} \xi = i/\ell, \tag{7.21}$$

where

$$\ell = \left[\frac{(b_{11}c_{11} - d_{11}^2)\epsilon_0}{(1 + \epsilon_0 a_{11})c_{11}}\right]^{1/2}. \tag{7.22}$$

If the contribution of the polarization gradient is omitted, b_{11} and d_{11} are zero and (7.16) reduces to

$$\begin{aligned} c_{11}\partial_1^2 u_1 &= \rho\ddot{u}_1, \\ a_{11}P_1 + \partial\varphi &= 0, \\ -\epsilon_0\partial_1^2\varphi + \partial P_1 &= 0, \end{aligned} \tag{7.23}$$

which is Toupin's form of the classical equations for the one-dimensional, linear, centrosymmetric case. In (7.23), there is no electromechanical coupling; the wave motion is dispersionless with frequency given by (7.20) for all ξ.

If, again, the contribution of the polarization gradient is omitted but the material is non-centrosymmetric, (7.23) becomes

$$
\begin{aligned}
c_{11}\partial_1^2 u_1 + f_{11}\partial_1 P_1 &= \rho\ddot{u}_1 , \\
f_{11}\partial_1 u_1 + a_{11} P_1 + \partial_1\varphi &= 0, \\
-\epsilon_0\partial_1^2\varphi + \partial_1 P_1 &= 0,
\end{aligned}
\tag{7.24}
$$

so that electromechanical coupling is regained. Inserting (7.11) in (7.24) and eliminating A, B and C, we find

$$
\rho\omega^2 = [c_{11} - f_{11}^2/(a_{11} + \epsilon_0^{-1})]\xi^2 . \tag{7.25}
$$

Thus, even though non centrosymmetry induces electromechanical coupling, there is still no imaginary branch and the real branch is dispersionless — in the absence of the contribution of the polarization gradient.

8. Monatomic Lattice of Shell-Model Atoms

In this Article, the difference equations of motion are derived for a one-dimensional, monatomic lattice of the Cochran type [46] based on the Dick-Overhauser [47] shell-model of the atom: a core, comprising the nucleus and inner electrons, surrounded by a shell of outer electrons. The electronic polarization is proportional to the relative displacement of the core and shell of the atom. In addition to this intra-atomic interaction, account is taken of interatomic interactions between core and core, core and shell and shell and shell of nearest neighbor atoms. It is shown that the equations of the lattice have, as their continuum limit, the augmented equations [44] described in the preceding Article rather than the equations of the classical theory of elastic dielectrics. The additional effects associated with the new material constants b_{ijkl} and d_{ijkl} stem primarily from the shell-shell interaction. This interaction is known to be important in the matching of lattice dispersion relations to dispersion data from neutron diffraction measurements at short wave lengths [26,48].

We consider a single line of atoms (Fig. 12) extracted from a three-dimensional, monatomic lattice of shell-model atoms. The atoms are situated at $x_1 = na$ where n is a positive or negative integer and a is the lattice parameter. The displacements of the core and shell of the atom at $x_1 = na$ are designated by u_n and s_n, respectively. The force constant of the intra-atomic core-shell interaction is designated by α and the force constants of the interatomic core-core, core-shell and shell-shell interactions are designated by β, γ and δ, respectively.

The equation of motion of the n^{th} interior atom (core and shell combined) is obtained by setting the inertia of the atom equal to the sum of the forces on its core and shell by the cores and shells of its two nearest neighbor atoms:

$$\begin{aligned}&\beta(u_{n+1}-u_n)+\gamma(s_{n+1}-u_n)+\gamma(u_{n+1}-s_n)+\delta(s_{n+1}-s_n)\\&-\beta(u_n-u_{n-1})-\gamma(u_n-s_{n-1})-\gamma(s_n-u_{n-1})-\delta(s_n-s_{n-1})=m\ddot{u}_n,\end{aligned} \tag{8.1}$$

where m is the mass of the atom. The shell, alone, of the n^{th} atom is acted upon by its own core, the core and shell of each of the two neighboring atoms and, also, the Maxwell, electric self-field (which occupies all space). Hence

$$\alpha(u_n - s_n) + \gamma(u_{n+1} - s_n) + \delta(s_{n+1} - s_n)$$
$$- \gamma(s_n - u_{n-1}) - \delta(s_n - s_{n-1}) + q E_n = 0, \tag{8.2}$$

in which the inertia of the shell is neglected, q is the charge of the atom and E_n is the value, at $x_1 = na$, of the Maxwell field. Now, $E_n = -[\partial_1 \varphi]_{x_1=na}$ and this may be expressed in terms of φ_n, the value of the potential φ at $x_1 = na$, by expanding the derivative in an infinite series of forward differences [7]:

$$E_n = \partial^+ \varphi_n = \sum_{m=1}^{\infty} (-1)^{m-1} m^{-1} a^{m-1} \Delta_+^m \varphi_n, \tag{8.3}$$

where

$$\begin{aligned}
\Delta_+ \varphi_n &= (\varphi_{n+1} - \varphi_n)/a, \\
\Delta_+^2 \varphi_n &= (\varphi_{n+2} - 2\varphi_{n+1} + \varphi_n)/a^2 \\
\Delta_+^3 \varphi_n &= (\varphi_{n+3} - 3\varphi_{n+2} + 3\varphi_{n+1} - \varphi_n)/a^3 \\
&\vdots \qquad\qquad \vdots
\end{aligned} \tag{8.4}$$

The polarization of the n^{th} atom, per unit area of the three dimensional lattice, is defined by

$$P_n = (s_n - u_n) q / a^3. \tag{8.5}$$

Then the equations of motion (8.1) and (8.2) may be rearranged to the following forms:

$$\begin{aligned}
(\beta + 2\gamma + \delta) a^{-1} \Delta_1^2 u_n + (\gamma + \delta) a^2 q^{-1} \Delta_1^2 P_n &= \rho \ddot{u}_n, \\
(\gamma + \delta) a^2 q^{-1} \Delta_1^2 u_n + \delta a^5 q^{-2} \Delta_1^2 P_n - (\alpha + 2\gamma) a^3 q^{-2} P_n - \partial^+ \varphi_n &= 0,
\end{aligned} \tag{8.6}$$

where $\rho = m/a^3$ and Δ_1^2 is the second central difference operator (divided by a^2) as defined in (2.3).

It will be observed that the difference equations (8.6) have the same form as the first two of (7.16), which are the one-dimensional differential equation of motion of the augmented theory of elastic dielectrics. Accordingly, if we set

$$a_{11} = (\alpha + 2\gamma)a^3 q^{-2} = \epsilon_0^{-1}\eta^{-1}, \qquad b_{11} = \delta a^5 q^{-2},$$
$$c_{11} = (\beta + 2\gamma + \delta)a^{-1}, \qquad d_{11} = (\gamma + \delta)a^2 q^{-1} \tag{8.7}$$

and employ the expansion (2.7) of the second central difference in series of derivatives, we find that the first two of (7.16) are the lowest order continuum approximation to the equations of motion of the atom and its shell, respectively.

As may be seen from (8.1) the polarization gradient terms (those with coefficients b_{11} and d_{11}) in (7.16) stem from the shell-shell and interatomic core-shell interactions — identified by the force constants δ and γ, respectively. In fact, the form of (7.16) is preserved if the interatomic core shell interaction is omitted but the shell-shell interaction is retained. If both of these interactions are omitted, the continuum approximation reduces to (7.17), which is Toupin's form of the classical equations (in the one-dimensional, linear case). The second of (7.17), Toupin's "equation of intramolecular force balance", does not appear in the traditional equations of elastic dielectrics; but we see that it is a fundamental equilibrium condition: the equilibrium of the shell (i.e. the outer electrons) under the action of the core of the same atom and the surrounding Maxwell field. The corresponding equation in the extended theory (the second of (7.16)) includes, in addition, the action of the adjacent atoms on the shell (in the continuum approximation).

We have yet to derive the lattice counterpart of the third of (7.16) (the "charge equation") and establish the boundary conditions. It is illuminating to reach these results from considerations of energy.

By analogy with (6.12) and (7.8), let us take, for the electric enthalpy of the one-dimensional lattice (per unit volume a^3)

$$\mathcal{H} = \sum_n \left[b_0 \Delta_+ P_n + \tfrac{1}{2}\epsilon_0^{-1}\eta^{-1} P_n^2 + \tfrac{1}{2} b_{11}(\Delta_+ P_n)^2 + c_{11}(\Delta_+ u_n)^2 \right.$$
$$\left. + d_{11}(\Delta_+ P_n)(\Delta_+ u_n) - \tfrac{1}{2}\epsilon_0 (\partial^+\varphi_n)^2 + P_n(\partial^+\varphi_n)\right]. \qquad (8.3)$$

We have to find the derivatives of $\mathcal{H}$ with respect to u_n, P_n and φ_n. The first two are conventional and straightforward. For example,

$$\frac{\partial(\Delta_+ u_m)^2}{\partial u_n} = \frac{1}{a^2}\,\frac{\partial(u_{m+1}-u_m)^2}{\partial u_n} = \frac{2}{a^2}(u_{m+1}-u_m)\,\frac{\partial(u_{m+1}-u_m)}{\partial u_n},$$
$$= \frac{2}{a^2}(u_{m+1}-u_m)(\delta_n^{m+1}-\delta_n^m),$$
$$= \frac{2}{a^2}(u_n - u_{n-1} - u_{n+1} - u_n) = 2\Delta_1^2 u_n, \qquad (8.9)$$

where δ_q^p is the Kronecker delta. To find the derivative of $\partial^+\varphi$ with respect to φ_n, note first that, from (8.3),

$$\partial^+\varphi_n = a^{-1}\left[\varphi_{n+1}\cdot\varphi_n - \tfrac{1}{2}(\varphi_{n+2}-2\varphi_{n+1}+\varphi_n)\right.$$
$$\left. + \tfrac{1}{3}(\varphi_{n+3}-3\varphi_{n+2}+3\varphi_{n+1}-\varphi_n) - \dots\right].$$

Then

$$P_m\frac{\partial(\partial^+\varphi_m)}{\partial\varphi_n} = a^{-1}P_m\left[\delta_n^{m+1}-\delta_n^m - \tfrac{1}{2}(\delta_n^{m+2}-2\delta_n^{m+1}+\delta_n^m)\right.$$
$$\left. + \tfrac{1}{3}(\delta_n^{m+3}-3\delta_n^{m+2}+3\delta_n^{m+1}-\delta_n^m) - \dots\right],$$
$$= a^{-1}\left[P_{n-1}-P_n - \tfrac{1}{2}(P_{n-2}-2P_{n-1}+P_n)\right.$$
$$\left. + \tfrac{1}{3}(P_{n-3}-3P_{n-2}+3P_{n-1}-P_n) - \dots\right],$$
$$= -\partial^- P_n, \qquad (8.10)$$

where

$$\partial^- P_n = \sum_{m=1}^{\infty} m^{-1} a^{m-1}\Delta_-^m P_n \qquad (8.11)$$

and

$$\Delta_- P_n = (P_n - P_{n-1})/a,$$
$$\Delta_-^2 P_n = (P_n - 2P_{n-1} + P_{n-2})/a^2, \qquad (8.12)$$
$$\Delta_-^3 P_n = (P_n - 3P_{n-1} + 3P_{n-2} - P_{n-3})/a^3,$$
$$\vdots \qquad\qquad \vdots$$

i.e. $\partial^- P_n$ is the expansion of $\partial_1 P$ in an infinite series of backward differences [7]. Finally

$$\frac{\partial(\partial^+\varphi_m)^2}{\partial\varphi_n} = 2\partial^+\varphi_m \frac{\partial(\partial^+\varphi_m)}{\partial\varphi_n} = -2\partial^-\partial^+\varphi_n . \tag{8.13}$$

We now find the equations of motion:

$$\begin{aligned}
-\frac{\partial H}{\partial u_n} &= c_{11}\Delta_1^2 u_n + d_{11}\Delta_1^2 P_n = \rho\ddot{u}_n ,\\
-\frac{\partial H}{\partial P_n} &= d_{11}\Delta_1^2 u_n + b_{11}\Delta_1^2 P_n - \epsilon_0^{-1}\eta^{-1}P_n - \partial^+\varphi_n = 0 ,\\
-\frac{\partial H}{\partial\varphi_n} &= -\epsilon_0\partial^-\partial^+\varphi_n + \partial^- P_n = 0.
\end{aligned} \tag{8.14}$$

The first two of (8.14) are the same as (8.6), with (8.7). This justifies the assumption (8.8) for the electric enthalpy. Also, we have found the third of (8.14), which has the third of (7.16) as its continuum form.

If the lattice is of finite thickness spanning an odd number of atoms with the end ones at $n = \pm N$, the conditions for free boundaries are

$$\begin{aligned}
-\frac{\partial H}{\partial(\Delta_+ u_{\pm N})} &= c_{11}\Delta_+ u_{\pm N} + d_{11}\Delta_+ P_{\pm N} = 0,\\
-\frac{\partial H}{\partial(\Delta_+ P_{\pm N})} &= d_{11}\Delta_+ u_{\pm N} + b_{11}\Delta_+ P_{\pm N} + b_0 = 0,\\
-\frac{\partial H}{\partial(\partial^+\varphi_{\pm N})} &= \epsilon_0\partial^+\varphi_{\pm N} - P_{\pm N} = 0,
\end{aligned} \tag{8.15}$$

where

$$\Delta_+ f_{\pm N} = (f_{\pm(N+1)} - f_N)/a , \quad \partial^+\varphi_{\pm N} = (\partial^+\varphi_n)_{n=\pm N}. \tag{8.16}$$

In general, admissible boundary conditions are: the specification of one member of each of the three products, at each end,

$$u_{\pm N}(c_{11}\Delta_+ u_{\pm N} + d_{11}\Delta_+ P_{\pm N}),\ P_{\pm N}(d_{11}\Delta_+ u_{\pm N} + b_{11}\Delta_+ P_{\pm N} + b_0),\ \varphi_{\pm N}(\epsilon_0\partial^+\varphi_{\pm N} - P_{\pm N});$$

i.e. eight possible combinations at each end, for the one-dimensional case.

The dispersion relation for (8.14) is obtained by inserting the functions

$$u_n = Ae^{i(\xi na-\omega t)}, \quad P_n = Be^{i(\xi na-\omega t)}, \quad \varphi_n = Ce^{i(\xi na-\omega t)} \tag{8.17}$$

in the equations and eliminating A, B and C, with the result

$$\begin{vmatrix} 2a^{-2}c_{11}(1-\cos\xi a)-\rho\omega^2 & 2a^{-2}d_{11}(1-\cos\xi a) \\ 2a^{-2}d_{11}(1-\cos\xi a) & 2a^{-2}b_{11}(1-\cos\xi a)+a_{11}+\epsilon_0^{-1} \end{vmatrix} = 0. \tag{8.18}$$

This two-branch dispersion relation is to be compared with (7.18) — the dispersion relation for the long wave approximation. For $\xi a \ll 1$ and real,

$$2a^{-2}(1-\cos\xi a) \to \xi^2,$$

so that (8.18) reduces to (7.18), as expected. Thus, the long wave behavior of the real branch of (8.18) is again given by (7.20). As for the imaginary branch of (8.18), the wave number at zero frequency is given by

$$\sin\frac{\xi a}{2} = \frac{ia}{2\ell}; \text{ or } \xi a = \frac{ia}{\Lambda}, \text{ where } \sinh\frac{a}{2\Lambda} = \frac{a}{2\ell}, \tag{8.19}$$

instead of $\xi a = ia/\ell$. That is, although the low frequency ends of the branches for the long wave approximation (7.18) are qualitatively the same as the low frequency limit of the branches for the lattice, only the real branches are quantitatively the same there (Fig. 13). The limit of the imaginary branch for the long wave approximation is somewhat in error, as the wave number at $\omega = 0$ is not small. Typically, a/ℓ might range between 1 and 2; then the error in the continuum approximation $\xi a = ia/\ell$, as compared with ia/Λ, would range from 4% to 12% — on the large side. As will be seen, the imaginary wave number is associated with surface effects not found in the classical theory; and an error in the wave number affects the amplitude of these effects and their spatial rate of decay into the interior.

The range of a/ℓ from 1 to 2 stems from calculations, by Askar, Lee and Cakmak [49], of the values of the new constants b_{11} and d_{11} (and, consequently, ℓ) for several alkali halide crystals. They found the relations of these constants to the constants in a three-dimensional Cochran [46] lattice of Dick-Overhauser [47] shell-model atoms in an NaCl structure. The correspondence is not complete because the NaCl lattice is diatomic whereas the continuum in Article 1 is a simple (i.e. not compound) one. However the long wave, low frequency limit of the lattice equations has the same form as the continuum equations in Article 1.

9. Capacitance of Thin, Dielectric Films

The example of the electrical capacitance of thin, dielectric films supplies a vehicle suitable for comparisons of experimental data with the predictions of the classical theory of elastic dielectrics, polarization gradient theory and lattice theory.

Consider a metal-dielectric-metal sandwich whose middle plane x_2-x_3, is a plane of geometrical and material symmetry. If end effects are neglected, the fields are one-dimensional and the equations of equilibrium are given by (7.16) with $\ddot{u}_1 = 0$.

Let us first solve the problem within the framework of the classical theory. Then b_{11} and d_{11} are zero and the equations of equilibrium reduce to (7.23) with $\ddot{u}_1 = 0$:

$$c_{11}\partial_1^2 u_1 = 0, \quad a_{11}P_1 + \partial_1\varphi = 0, \quad -\epsilon_0\partial_1^2\varphi + \partial_1 P_1 = 0. \tag{9.1}$$

For a dielectric layer with traction-free surfaces at $x_1 = \pm h$, on which are impressed voltages $\pm V$, the boundary conditions, according to the classical theory, are

$$[\partial_1 u_1]_{x_1=\pm h} = 0, \qquad [\varphi]_{x_1=\pm h} = \pm V; \tag{9.2}$$

and the solution of (9.1), subject to these boundary conditions, is, except for additive constants in u_1 and φ,

$$u_1 = 0, \quad P_1 = -\epsilon_0\eta V/h, \quad \varphi = Vx_1/h, \tag{9.3}$$

where $\eta, = \epsilon_0^{-1}a_{11}^{-1}$, is the dielectric susceptibility.

The capacitance (per unit area) is the ratio of the surface charge (per unit area) to the voltage drop across the layer:

$$C = \frac{[\epsilon_0\partial\varphi - P_1]_{x_1=\pm h}}{2V} = \frac{\epsilon_0(1+\eta)}{2h} = \frac{\epsilon}{2h}, \tag{9.4}$$

where ϵ is the permittivity of the dielectric.

Thus, according to the classical theory, there is no strain, the polarization is uniform, the potential varies linearly through the thickness and the capacitance is inversely proportional to the thickness, so that a graph of inverse capacitance vs. thickness is a straight line through the origin. However, in a series of experiments with a variety of very thin dielectric films between metal electrodes, Mead [50, 51, 52] found a different relation between inverse capacitance and thickness. His experimental data fall on straight lines which, if extended to zero thickness, have positive intercepts of inverse capacitance, as illustrated in Fig. 14. Initially [50], Mead suggested that the anomaly might be due to penetration of the field into the electrodes; but subsequently [51] he abandoned that view, although, meanwhile, it had been supported by Ku and Ullman [52]. An alternative explanation is found in the augmented theory of elastic dielectrics [53].

The solution of the augmented equations of equilibrium, (1.16) with $\ddot{u}_1 = 0$, analogous to the one just given for the classical equations, requires a boundary condition in addition to the surface traction and potential. The additional condition can be the specification of the polarization at the surface of the dielectric. Now, the polarization at a boundary of the dielectric in a metal-dielectric-metal sandwich will depend on the physical properties of the adjacent electrode and metal-dielectric interface; and these properties are outside the compass of the theory of dielectrics. However, since the polarization in the metal is zero, it is reasonable to assume that the surface polarization in the dielectric, if not actually zero, will lie between zero and the classical value given by the second of (9.3). Thus, assuming that the two electrodes and interfaces are the same, their influence on the surface polarization may be introduced, phenomenologically, by setting the boundary condition

$$[P_1]_{x_1=\pm h} = -k\epsilon_0\eta V/h, \qquad 0 \leq k \leq 1, \tag{9.5a}$$

The classical condition is $k=1$ while $k=0$ describes continuity of polarization across the interfaces. We suppose also, as is assumed in the classical theory, that the traction across the interfaces is zero. From (1.15), this condition is

$$[T_{11}]_{x_1=\pm h} = [c_{11}\partial_1 u_1 + d_{11}\partial_1 P_1]_{x_1=\pm h} = 0. \tag{9.5b}$$

Finally, we suppose that the voltages applied to the dielectric at the interfaces are again

$$[\varphi]_{x_1=\pm h} = \pm V. \tag{9.5c}$$

We have now to solve (7.16), with $\ddot{u}_1 = 0$, subject to the boundary conditions (9.5a, b, c). Let

$$u_1 = B_1 \cosh\frac{x_1}{\ell}, \quad P_1 = A_2 + B_2\cosh\frac{x_1}{\ell}, \quad \varphi = A_3 x_1 + B_3 \sinh\frac{x_1}{\ell}. \tag{9.6}$$

Upon substituting (9.6) in (1.16), we find

$$A_2 = \epsilon_0\eta A_3, \quad B_3 = \ell B_2/\epsilon_0 = -\ell c_{11} B_1/\epsilon_0 d_{11}, \tag{9.7}$$

where

$$\ell = \left(\frac{b_{11}c_{11} - d_{11}^2}{c_{11}(a_{11}+\epsilon_0^{-1})}\right)^{1/2} = \left(\frac{\epsilon_0(b_{11}c_{11}-d_{11}^2)}{c_{11}(1+\eta^{-1})}\right)^{1/2} \tag{9.8}$$

i.e. ℓ is the same as in (7.22).

As for boundary conditions, (9.5b) is satisfied identically while (9.5a) and (9.5c) become

$$\begin{aligned} A_2 + B_2\cosh(h/\ell) &= -k\epsilon_0\eta V/h, \\ A_3 h + B_3 \sinh(h/\ell) &= V, \end{aligned} \tag{9.9}$$

respectively. From (9.7) and (9.9),

$$\begin{aligned} A_3 &= (B_3/\eta\ell)\cosh(h/\ell) + kVh, \\ B_3 &= (1-k)\eta V/[\eta\sinh(h/\ell) + (h/\ell)\cosh(h/\ell)]. \end{aligned} \tag{9.10}$$

The remaining constants are obtained from (9.10) and (9.7).

The capacitance is

$$C = \frac{[\epsilon_0 \partial\varphi - P_1]_{x_1=\pm h}}{2V} = \frac{\epsilon}{2h}\,\frac{1+(k\eta\ell/h)\tanh(h/\ell)}{1+(\eta\ell/h)\tanh(h/\ell)}, \tag{9.11}$$

if we ignore any voltage drop that may occur in the electrodes.

In Fig. 15, the curve marked $k = 0.1$ shows the relation between normalized inverse capacitance and normalized thickness, according to (9.11), for the case $\eta = 10$, $k = 0.1$. Calculations from Mead's data, for small k, indicate that the material property ℓ for all his dielectrics is of the order of magnitude of a few angstroms; and this is supported by Askar, Lee and Cakmak's calculations for alkali halides [49]. Hence, Mead's data, which do not extend below a thickness of 30 Å, would be well to the right of the knee of the curve $k = 0.1$, in Fig. 15, and so would give the appearance of a linear relation which, if extended to zero thickness, would have a non-zero, positive, intercept of inverse capacitance. This intercept, according to (9.11), is

$$C_0^{-1} = 2\ell(1-k)\eta/\epsilon\,. \tag{9.12}$$

If $k = 1$, the intercept reduces to zero and, in fact, the whole solution reduces to the classical one. However, it seems unlikely that the presence of the metal would not influence the polarization of the dielectric at the metal-dielectric interface.

The polarization and potential vary across the thickness of the dielectric as shown in Fig. 16. The absolute value of the polarization is almost uniform across the major portion of the thickness and slightly less than the uniform polarization of the classical theory; but then drops sharply, near the surfaces, to boundary values k times the classical polarization, as specified. The potential has an almost uniform

gradient, less than the uniform gradient of the classical theory, over most of the thickness, but then increases sharply on approaching the boundaries. The extremely localized surface effects are accounted for by the contribution of the polarization gradient to the stored energy and are associated, mathematically, with the imaginary branch of the dispersion relation — a branch not present in the classical theory.

Now consider the analogous solution of the lattice equations (8.14), with $\ddot{u}_n = 0$, subject to boundary conditions analogous to (9.5):

$$P_{\pm N} = -k\epsilon_0 \eta V/h, \quad c_{11}\Delta_+ u_{\pm N} + d_{11}\Delta_+ P_{\pm N} = 0, \quad \varphi_{\pm N} = \pm V, \tag{9.13}$$

where $h = Na$. We take

$$u_n = B_1' \cosh\frac{na}{\lambda}, \quad P_n = A_2' + B_2' \cosh\frac{na}{\lambda}, \quad \varphi_n = A_3' na + B_3' \sinh\frac{na}{\lambda} \tag{9.14}$$

and note that $\partial^2 [f_n(na)] = [\partial_1 f(x_1)]_{x_1 = na}$ and

$$\Delta^2 \cosh\frac{na}{\lambda} = a^{-2}\left[\cosh\frac{(n+1)a}{\lambda} + \cosh\frac{(n-1)a}{\lambda} - 2\cosh\frac{na}{\lambda}\right] = 4a^{-2}\sinh^2\frac{a}{2\lambda}\cosh\frac{na}{\lambda}. \tag{9.15}$$

Then, substituting (9.14) in (8.14), we find, analogous to (9.7),

$$A_2' = \epsilon_0 \eta A_3', \quad B_3' = \lambda B_2'/\epsilon_0 = -\lambda c_{11} B_1'/\epsilon_0 d_{11} \tag{9.16}$$

and, in place of (9.8),

$$\sinh(a/2\lambda) = a/2\ell, \tag{9.17}$$

where ℓ is the same as in (9.8). Thus, (9.16) is the same as (9.7) with ℓ replaced by λ; but ℓ and λ are not quite the same: being related in accordance with (9.17) and differing by some 4 to 12 percent, as remarked following (8.19).

Application of the boundary conditions (9.13) leads, by the same procedure as for the continuum, to

$$A_3' = \frac{B_3'}{\eta\lambda}\cosh\frac{h}{\lambda} + \frac{kV}{h}, \quad B_3' = \frac{(1-k)\eta V}{\eta \sinh\frac{h}{\lambda} + \frac{h}{\lambda}\cosh\frac{h}{\lambda}}, \tag{9.18}$$

analogous to (9.10). Finally, the capacitance is

$$C = \frac{\epsilon_0 \partial^+ \varphi_{\pm N} - P_{\pm N}}{2V} = \frac{\epsilon}{2h} \frac{1 + (k\eta\lambda/h)\tanh(h/\lambda)}{1 + (\eta\lambda/h)\tanh(h/\lambda)} . \tag{9.19}$$

Thus, the entire solution is identical with the continuum one except that the displacement and polarization have significance only at the atom sites and ℓ is replaced by λ. In particular, the curve in Fig. 15 is applicable to the lattice if ℓ is replaced by λ in both abscissa and ordinate.

10. Surface Energy of Deformation and Polarization

It will be observed that the internal energy density of deformation and polarization, (7.8), contains the term $b^{\circ}_{ij} P_{j,i}$ linear in the polarization gradient. As remarked in Article 3, the analogous term linear in the strain, say $c^{\circ}_{ij} S_{ij}$, is omitted as it is of no consequence. It leads to a homogeneous stress which, in a bounded body with a free surface, can be removed by a homogeneous strain which, in turn, can be regarded as the reference configuration. The situation is otherwise for the term linear in the polarization gradient. Although this, too, produces a homogeneous field, it is a field of E_{ij} rather than T_{ij}, as may be seen by referring to the constitutive equations (7.9). The removal of $n_i E_{ij}$ to free a surfac· (see (7.7)) results, as is illustrated below, in a polarization and strain which decay exponentially into the interior of the body.

As is described in Article 3, the energy required to separate a body into two parts comprises a bond energy and a remainder. The former is what would be required to break the atomic bonds across the surface if the strain, and now the polarization, were prevented from developing, say by hypothetical mechanical and electrical external fields. The release of the hypothetical fields would result in a deformation and polarization, localized near the surface, with which is associated a surface energy of deformation and polarization — always negative. Thus, the energy required to separate a body into two parts is the bond energy less the absolute value of the surface energy of deformation and polarization. The latter is introduced by the linear term, $b^{\circ}_{ij} P_{j,i}$, in W^L and a formula for that part of the surface energy may be found as follows

The total energy in the system, in equilibrium, is

$$\int_{V^*} W\,dV = \int_{V^*} (W^L + \tfrac{1}{2}\epsilon_0 \varphi_{,i}\varphi_{,i})\,dV = \int_V W^L dV + \int_{V^*} \tfrac{1}{2}\epsilon_0 \varphi_{,i}\varphi_{,i}\,dV, \qquad (10.1)$$

where V is the volume occupied by the dielectric solid bounded by a surface S separating V from an outer vacuum V'; and $V^* = V + V'$.

By means of the constitutive equations (7.9), the form of W^L may be converted from (7.8) to

$$2W^L = T_{ij}S_{ij} + E_{ij}P_{j,i} - E_i^L P_i + b_{ij}^{\circ} P_{j,i}. \tag{10.2}$$

Through the use of the chain rule of differentiation and the divergence theorem,

$$\int_V T_{ij}S_{ij}\,dV = \int_V T_{ij}u_{j,i}\,dV = \int_V [(T_{ij}u_j)_{,i} - T_{ij,i}u_j]\,dV$$
$$= \int_S n_i T_{ij}u_j\,dS - \int_V T_{ij,i}u_j\,dV,$$

$$\int_V E_{ij}P_{j,i}\,dV = \int_V [(E_{ij}P_j)_{,i} - E_{ij,i}P_j]\,dV = \int_S n_i E_{ij}P_j\,dS - \int_V E_{ij,i}P_j\,dV,$$

$$\int_V b_{ij}^{\circ} P_{j,i}\,dV = \int_S n_i b_{ij}^{\circ} P_j\,dS,$$

$$\int_{V^*} \varphi_{,i}\varphi_{,i}\,dV = \int_{V^*} [(\varphi_{,i}\varphi)_{,i} - \varphi_{,ii}\varphi]\,dV$$
$$= \int_S n_i [\varphi_{,i}]\varphi\,dS - \int_V \varphi_{,ii}\varphi\,dV - \int_{V'} \varphi_{,ii}\varphi\,dV,$$

where $[\varphi_{,i}]$ is the jump in $\varphi_{,i}$ across S. Upon inserting these results in (10.1), we have

$$\int_{V^*} W\,dV = \tfrac{1}{2}\int_S n_i [b_{ij}^{\circ}P_j + T_{ij}u_j + E_{ij}P_j + \epsilon_0[\varphi_{,i}]\varphi]\,dS$$
$$- \tfrac{1}{2}\int_V (T_{ij,i}u_j + E_{ij,i}P_j + E_j^L P_j + \epsilon_0\varphi_{,ii}\varphi)\,dV - \int_{V'} \epsilon_0\varphi_{,ii}\varphi\,dV. \tag{10.3}$$

Application of the equilibrium equations, i.e. (7.5) and (7.6) with $\ddot{u}_j = 0$, to (10.3) reduces it to

$$\int_{V^*} W\,dV = \tfrac{1}{2}\int_V (f_j u_j + E_j^{\circ}P_j)\,dV + \tfrac{1}{2}\int_S n_i [T_{ij}u_j + E_{ij}P_j - (-\epsilon_0[\varphi_{,i}] + P_i) + b_{ij}^{\circ}P_j]\,dS. \tag{10.4}$$

Then, in the absence of external fields ($f_j = E_j^{\circ} = 0$) and with the boundary free, i.e. (7.7) with $t = 0$, (10.4) reduces to

$$\int_{V^*} W\,dV = \tfrac{1}{2}\int_S n_i b_{ij}^{\circ} P_j\,dS. \tag{10.5}$$

This is the energy of deformation and polarization which must be added to the bond energy to obtain the total energy required to separate the material along the surface S. As indicated by Schwartz [54], the additional energy is always negative as a consequence of the positive definiteness of the quadratic part of the energy density which, in turn, is required for stability — i.e. because energy must be stored, rather than generated, during the application of external body or surface forces. Thus,

$$\int_{V^*} W\,dV = \int_{V^*}\left[\tfrac{1}{2}\varphi_{,i}\varphi_{,i} + (W^L - b^\circ_{ij}P_{j,i})\right]dV + \int_V b^\circ_{ij}P_{j,i}\,dV$$

$$= \int_{V^*}\left[\tfrac{1}{2}\varphi_{,i}\varphi_{,i} + (W^L - b^\circ_{ij}P_{j,i})\right]dV + \int_S n_i b^\circ_{ij}P_j\,dS. \qquad (10.6)$$

Subtracting (10.5) from (10.6), we have

$$\int_{V^*}\left[\tfrac{1}{2}\varphi_{,i}\varphi_{,i} + (W^L - b^\circ_{ij}P_{j,i})\right]dV + \tfrac{1}{2}\int_S n_i b^\circ_{ij}P_j\,dS = 0. \qquad (10.7)$$

But the volume integral in (10.8) is positive. Hence

$$\int_S n_i b^\circ_{ij}P_j\,dS < 0. \qquad (10.8)$$

Finally, we may define

$$W^S = \tfrac{1}{2}\left[n_i b^\circ_{ij}P_j\right]_S \qquad (10.9)$$

as the surface energy of deformation and polarization per unit area, sometimes called the surface tension.

There follows the solution for the displacement, polarization, potential and surface energy of deformation and polarization in the half-space of a centrosymmetric cubic crystal bounded by a free (100) face. For this problem, the fields are one-dimensional and in equilibrium so that, for the half-space $x_1 = 0$, the equations of motion (7.15) reduce to

$$\begin{aligned} c_{11}\partial_1^2 u_1 + d_{11}\partial_1^2 P_1 &= 0, \\ d_{11}\partial_1^2 u_1 + b_{11}\partial_1^2 P_1 - a_{11}P_1 - \partial\varphi &= 0, \\ -\epsilon_0\partial_1^2\varphi + \partial_1 P_1 &= 0; \end{aligned} \qquad (10.10)$$

and the boundary conditions (7.7) become, on $x_1 = 0$,

$$
\begin{aligned}
c_{11}\partial_1 u_1 + d_{11}\partial_1 P_1 &= 0, \\
d_{11}\partial_1 u_1 + b_{11}\partial_1 P_1 &= -b_0, \\
-\epsilon_0 \partial_1 \varphi + P_1 &= 0.
\end{aligned}
\tag{10.11}
$$

Consider

$$
u_1 = A_1 e^{-x_1/\ell}, \quad P_1 = A_2 e^{-x_1/\ell}, \quad \varphi = A_3 e^{-x_1/\ell}. \tag{10.12}
$$

Upon substituting (10.12) into (10.10), we find

$$
A_3 = -\ell A_2/\epsilon_0 = \ell c_{11} A_1/\epsilon_0 d_{11} \tag{10.13}
$$

where ℓ is again given by (7.22). With (10.13), the first and third of the boundary conditions (10.11) are satisfied identically and the second boundary condition yields

$$
A_1 = -\frac{b_0 d_{11}}{c_{11}\ell(a_{11} + \epsilon_0^{-1})}. \tag{10.14}
$$

Then, from (10.13),

$$
A_2 = \frac{b_0}{\ell(a_{11}+\epsilon_0^{-1})}, \qquad A_3 = -\frac{b_0}{1+a_{11}\epsilon_0}. \tag{10.15}
$$

It may be seen that the freeing of the boundary results in a field of displacement, polarization and potential localized at the surface, decaying into the interior with decay constant ℓ. Associated with the localized field is a surface energy of deformation and polarization, per unit area, given by (10.9):

$$
W^S = -\frac{b_0^2}{2\ell a_{11}(1+a_{11}^{-1}\epsilon_0^{-1})}. \tag{10.16}
$$

Note that, from (6.26), (6.28) and (6.32),

$$
1 + a_{11}^{-1}\epsilon_0^{-1} = \epsilon_{11}^S/\epsilon_0 = \kappa_{11} \tag{10.17}
$$

i.e. the dielectric constant in the [100] direction.

As noted at the end of Article 8, Askar, Lee and Cakmak [49] have made calculations of the new material constants for several alkali halide crystals. From these they find, in the case of NaCl, for example,

$$\ell = 1.3 \times 10^{-8}\ \mathrm{cm}, \quad W^s = -59\ \mathrm{erg/cm^2}. \qquad (10.18)$$

The decay constant ℓ is about half the distance between nearest neighbor atoms in the NaCl crystal, indicating extremely rapid decay from the surface into the interior. The surface energy of deformation and polarization is about 30% of the bond energy, so that it is far from negligible. Both of these results conform to experimental observations [20, 21].

Additional solutions for surface energies of deformation and polarization (in isotropic materials) have been obtained by Schwartz [54] and by Askar, Lee and Cakmak [55] for internal spherical and cylindrical surfaces and a crack. The latter have used average values of their previous calculations of constants for alkali halides [49] to obtain some quantitative results. They find that the absolute values of W^s are reduced by curvature of internal surfaces and they also conclude that W^s is finite at the root of a crack.

11. Acoustical and Optical Activity in Alpha Quartz

Acoustical activity (rotation of the direction of mechanical displacement along the path of a transverse, elastic wave) has recently been observed by Pine [56] in α-quartz. The possibility of the phenomenon appears first to have been mentioned by Silin [57]. It was accounted for by Toupin [19] on the basis of the first strain gradient theory (Article 3ii). Portigal and Burstein [58] found an equivalent result by assigning dependence of the elastic stiffness on the wave vector. In the present article, it is shown [59] that both acoustical and optical activities are accounted for in the polarization gradient theory (Article 7). In what follows, the field equations are exhibited for the coupled elastic-electric-magnetic system, the problem of shear waves along the trigonal axis of α-quartz is solved, formulas are obtained for the optical and acoustical rotatory powers and numerical values of the new material constants, in the formulas, are calculated from experimental data. Essentially, the theory has it that the appearance of optical activity depends on an interaction between the polarization and the polarization gradient; the appearance of acoustical activity depends on interactions of the strain with both the polarization and the polarization gradient, and is absent if either interaction is missing.

When the magnetic field is taken into account, the equations of Article 7 become

$$T_{ij,i} + f_j = \rho \ddot{u}_j, \tag{11.1}$$

$$E_{ij,i} + E^L_j + E_j + E^0_j = 0, \tag{11.2}$$

$$\delta_{ijk} E_{k,j} + \dot{B}_i = 0, \tag{11.3}$$

$$\mu_0^{-1} \delta_{ijk} B_{k,j} - \epsilon_0 \dot{E}_i - \dot{P}_i = 0, \tag{11.4}$$

$$\epsilon_0 E_{i,i} + P_{i,i} = 0, \tag{11.5}$$

$$B_{i,i} = 0, \tag{11.6}$$

where B_i is the magnetic flux density, μ_0 is the magnetic permeability of a vacuum and δ_{ijk} is the unit alternating tensor. Also, as before,

$$T_{ij} = \frac{\partial W^L}{\partial S_{ij}}, \qquad E^L_i = -\frac{\partial W^L}{\partial P_i}, \qquad E_{ij} = \frac{\partial W^L}{\partial P_{j,i}}, \tag{11.7}$$

where

$$W^L = \tfrac{1}{2}a_{ij}P_iP_j + \tfrac{1}{2}b_{ijkl}P_{j,i}P_{l,k} + \tfrac{1}{2}c^P_{ijkl}S_{ij}S_{kl} + d_{ijkl}P_{j,i}S_{kl} + f_{ijk}P_iS_{jk} + j_{ijk}P_iP_{k,j}, \tag{11.8}$$

$$S_{ij} = \tfrac{1}{2}(u_{j,i} + u_{i,j}). \tag{11.9}$$

It is convenient to eliminate B_i at the start — by subtracting the curl of (11.3) from the time derivative of (11.4), with the result:

$$E_{j,ii} - E_{i,ij} = \epsilon_0\mu_0\ddot{E}_j + \mu_0\ddot{P}_j. \tag{11.10}$$

Equations (11.5) and (11.6) are not independent of (11.4) and (11.3), respectively, and may be disregarded for the present purpose. Thus, (11.10), along with (11.1) and (11.2):

$$\begin{aligned} T_{ij,i} + f_j &= \rho\ddot{u}_j, \\ E_{ij,i} + E^L_j + E_j + E^0_j &= 0, \\ E_{j,ii} - E_{i,ji} &= \epsilon_0\mu_0\ddot{E}_j + \mu_0\ddot{P}_j, \end{aligned} \tag{11.11}$$

are the field equations governing mechanical and electromagnetic waves, coupled through the constitutive equations:

$$\begin{aligned} T_{ij} &= c^P_{ijkl}S_{kl} + f_{kij}P_k + d_{klij}P_{l,k}, \\ -E^L_j &= f_{jkl}S_{kl} + a_{jk}P_k + j_{jkl}P_{l,k}, \\ E_{ij} &= d_{ijkl}S_{kl} + j_{kij}P_k + b_{ijkl}P_{l,k}, \end{aligned} \tag{11.12}$$

which are obtained from (11.7) and (11.8).

We consider plane, transverse waves propagating along the x_3-axis; i.e. u_3, P_3 and E_3 are zero and the remaining u_i, P_i, and E_i are functions of x_3 and t only. Then the field equations (11.11), with f_j and E^0_j zero, reduce to

$$\begin{aligned} T_{13,3} &= \rho\ddot{u}_1, & T_{23,} &= \rho\ddot{u}_2, \\ E_{31,3} + E^L_1 + E_1 &= 0, & E_{32,3} + E^L_2 + E_2 &= 0, \\ E_{1,33} &= \epsilon_0\mu_0\ddot{E}_1 + \mu_0\ddot{P}_1, & E_{2,33} &= \epsilon_0\mu_0\ddot{E}_2 + \mu_0\ddot{P}_2, \end{aligned} \tag{11.13}$$

and the constitutive equations (11.12) reduce to [59]

$$
\begin{aligned}
T_{31} &= c^P_{44} u_{1,3} - f_{14} P_2 + d_{74} P_{1,3}, & T_{32} &= c^P_{44} u_{2,3} + f_{14} P_1 + d_{74} P_{2,3}, \\
-E^L_1 &= f_{14} u_{2,3} + \epsilon_0^{-1}\chi_{11} P_1 + j_{17} P_{2,3}, & -E^L_2 &= -f_{14} u_{1,3} + \epsilon_0^{-1}\chi_{11} P_2 - j_{17} P_{1,3}, \\
E_{31} &= d_{74} u_{1,3} - j_{17} P_2 + b_{55} P_{1,3}, & E_{32} &= d_{74} u_{2,3} + j_{17} P_1 + b_{55} P_{2,3}
\end{aligned}
\tag{11.14}
$$

for the crystal class 32 (International) or D_3 (Schoenflies) [60] to which α-quartz belongs. In (11.14), the abridged notation

$$11 \to 1,\ 22 \to 2,\ 33 \to 3,\ 23 \to 4,\ 32 \to 7,\ 31 \to 5,\ 13 \to 8,\ 12 \to 6,\ 21 \to 9$$

is used for the subscripts attached to the material constants.

Inserting (11.14) in (11.13), we have

$$
\begin{aligned}
c^P_{44} u_{1,33} - f_{14} P_{2,3} + d_{74} P_{1,33} &= \rho \ddot{u}_1, \\
c^P_{44} u_{2,33} + f_{14} P_{1,3} + d_{74} P_{2,33} &= \rho \ddot{u}_2, \\
d_{74} u_{1,33} - 2 j_{17} P_{2,3} + b_{55} P_{1,33} - f_{14} u_{2,3} - \epsilon_0^{-1}\chi_{11} P_1 + E_1 &= 0, \\
d_{74} u_{2,33} + 2 j_{17} P_{1,3} + b_{55} P_{2,33} + f_{14} u_{1,3} - \epsilon_0^{-1}\chi_{11} P_2 + E_2 &= 0, \\
E_{1,33} &= \epsilon_0 \mu_0 \ddot{E}_1 + \mu_0 \ddot{P}_1, \\
E_{2,33} &= \epsilon_0 \mu_0 \ddot{E}_2 + \mu_0 \ddot{P}_2 .
\end{aligned}
\tag{11.15}
$$

Now, take

$$
\begin{aligned}
u_1 &= A_1 \sin\zeta(x_3 - vt), & u_2 &= A_2 \cos\zeta(x_3 - vt), \\
P_1 &= B_1 \sin\zeta(x_3 - vt), & P_2 &= B_2 \cos\zeta(x_3 - vt), \\
E_1 &= C_1 \sin\zeta(x_3 - vt), & E_2 &= C_2 \cos\zeta(x_3 - vt)
\end{aligned}
\tag{11.16}
$$

and substitute these functions in (11.15) to find

$$
\begin{aligned}
(c^P_{44} - \rho v^2)\zeta A_1 - f_{14} B_2 + d_{74}\zeta B_1 &= 0, \\
(c^P_{44} - \rho v^2)\zeta A_2 - f_{14} B_1 + d_{74}\zeta B_2 &= 0, \\
d_{74}\zeta^2 A_1 - f_{14}\zeta A_2 + (b_{55}\zeta^2 + \epsilon_0^{-1}\chi_{11}) B_1 - 2 j_{17}\zeta B_2 - C_1 &= 0, \\
d_{74}\zeta^2 A_2 - f_{14}\zeta A_1 + (b_{55}\zeta^2 + \epsilon_0^{-1}\chi_{11}) B_2 - 2 j_{17}\zeta B_1 - C_2 &= 0, \\
\mu_0 v^2 B_1 + (\epsilon_0 \mu_0 v^2 - 1) C_1 &= 0, \\
\mu_0 v^2 B_2 + (\epsilon_0 \mu_0 v^2 - 1) C_2 &= 0.
\end{aligned}
\tag{11.17}
$$

Adding and subtracting these equations in pairs, we have

$$
\begin{gathered}
(c_{44}^{p}-\rho v^2)(A_1\pm A_2)+(d_{74}\zeta\mp f_{14})(B_1\pm B_2)=0,\\
(d_{74}\zeta\mp f_{14})(A_1\pm A_2)+(b_{55}\zeta^2+\epsilon_0^{-1}\chi_{11}\mp 2j_{17}\zeta)(B_1\pm B_2)-(C_1\pm C_2)=0,\\
\mu_0 v^2(B_1\pm B_2)+(\epsilon_0\mu_0 v^2-1)(C_1\pm C_2)=0.
\end{gathered}
\tag{11.18}
$$

Thus, there are two solutions, each corresponding to circularly polarized waves [61, p.222] since the amplitudes must satisfy

$$
A_1=\pm A_2,\quad B_1=\pm B_2,\quad C_1=\pm C_2 \tag{11.19}
$$

with either all upper signs or all lower signs. Upon substituting (11.19) into (11.16), we see that the upper and lower signs give right and left circular polarization, respectively. The equation for the velocities is obtained by setting the determinant of the coefficients of the amplitudes in (11.18) equal to zero:

$$
\begin{vmatrix}
c_{44}^{p}-\rho v^2 & d_{74}\zeta\mp f_{14} & 0\\
d_{74}\zeta\mp f_{14} & b_{55}\zeta^2+\epsilon_0^{-1}\chi_{11}\mp 2j_{17}\zeta & 1\\
0 & 1 & \mu_0^{-1}v^{-2}-\epsilon_0
\end{vmatrix}=0. \tag{11.20}
$$

This is a quadratic equation in v^2, so that there are two pairs of oppositely circularly polarized waves. Each pair of such waves combines to produce a linearly polarized wave with a rotating direction of polarization [61, p.222]. Thus, we have two cases of rotary polarization. These may be identified as optical and acoustical by separating out first the electromagnetic part of (11.20) and then the electromechanical part. The two may, in fact, be considered separately owing to the large ratio of frequencies (of the order of 10^5) at which the two effects are observed.

The electromagnetic part of the determinant in (11.20) is the minor of the upper left element. Thus, the pair of optical velocities is given by

$$\begin{vmatrix} b_{55}\zeta^2 + \epsilon_0^{-1}\chi_{11} \mp 2 j_{17} & 1 \\ 1 & \mu_0 \quad {}^{-2} - \epsilon_0 \end{vmatrix} = 0, \tag{II.21}$$

which yields the dispersion formula [61, p.426]

$$n_\pm^2 - 1 = (\chi_{11} \mp 2\epsilon_0 j_{17}\zeta + \epsilon_0 b_{55}\zeta^2)^{-1}, \tag{II.22}$$

where $n_\pm$ are the indexes of refraction:

$$n_\pm = c/v_\pm \tag{II.23}$$

and c is the velocity of light in vacuo:

$$c = (\epsilon_0\mu_0)^{-1}. \tag{II.24}$$

From (II.22), we have

$$(n_-^2 - 1)^{-1} - (n_+^2 - 1)^{-1} = 4\epsilon_0 j_{17}\zeta. \tag{II.25}$$

Now, define $n = \frac{1}{2}(n_+ + n_-)$ and assume

$$|n_+ - n_-| \ll n_+ + n_-. \tag{II.26}$$

Then (II.25) becomes, approximately,

$$n_+ - n_- = 2(n^2-1)^2\epsilon_0 j_{17}\zeta_0, \tag{II.27}$$

where $\zeta_0, = \zeta/n,$ is the wave number in vacuo.

The optical rotatory power, in radians per unit length, is given by [61, p.222]

$$\theta_{op} = \tfrac{1}{2}\zeta_0(n_- - n_+). \tag{II.28}$$

Accordingly, from (II.27) and (II.28),

$$\theta_{op} = -(n^2-1)^2\epsilon_0 j_{17}\zeta_0^2 \tag{II.29}$$

is the formula for the optical rotatory power in terms of the average

index of refraction, n, along the optic axis, the wave length in vacuo, λ_0, $= 2\pi/\zeta_0$, the fundamental constant ϵ_0 and the material constan $j_{173} = j_{132}$, which, as may be seen in (11.8), measures the interaction between the polarization and the polarization gradient.

The electromechanical part of the determinant in (11.20) is the minor of the lower right element, so that we have

$$\begin{vmatrix} c^P_{44} - \rho v^2 & d_{74}\zeta \mp f_{14} \\ d_{74}\zeta \mp f_{14} & b_{55}\zeta^2 + \epsilon_0^{-1}\chi_{11} \mp 2j_{17}\zeta \end{vmatrix} = 0 \qquad (11.30)$$

for the equation determining the velocities of the two acoustical waves, as influenced by the quasi-static polarization and polarization gradient. From (11.30),

$$\rho v_\pm^2 = c^P_{44} - (d_{74}\zeta \mp f_{14})^2 / (b_{55}\zeta^2 + \epsilon_0^{-1}\chi_{11} \mp 2j_{17}\zeta). \qquad (11.31)$$

In view of (11.19) and the inequality of v_+ and v_-, the superposition of the two waves results in rotary polarization (acoustical activity) with acoustical rotatory power

$$\theta_{AC} = \tfrac{1}{2}\omega(v_-^{-1} - v_+^{-1}) \qquad (11.32)$$

where ω is the circular frequency. Both waves are dispersive. At the zero frequency (long wave) limit, from (11.31) and (6.34), with (6.28),

$$\lim_{\zeta\to 0} \rho v_\pm^2 = c^P_{44} - \epsilon_0 f_{14}^2/\chi_{11} = c^E_{44}, \qquad (11.33)$$

which is the result (without acoustical activity, since $v_+ = v_-$) that would be obtained if the contribution of the polarization gradient were omitted, i.e. if d_{74}, b_{55} and j_{17} were assumed to be zero. As the frequency increases from zero, the absolute velocity difference, $|v_+ - v_-|$, at first increases; so that the acoustical activity appears and increases. With further increase of frequency, the velocity difference again approaches zero, since

$$\lim_{\zeta\to\infty} \rho v_\pm^2 = c^P_{44} - d_{74}^2/b_{55}, \qquad (11.34)$$

so that the acoustical activity diminishes; but this is undoubtedly beyond the range of applicability of the continuum theory. Up to moderately large wave numbers, (11.31), with (6.28) and (6.34), gives, to the first order in ξ,

$$v_0/v_\pm = 1 \mp (d_{74} - j_{17}e_{14})e_{14}\xi/c^E_{44}\,, \tag{11.35}$$

where $v_0^2 = c^E_{44}/\rho$. In this range, the frequency is approximately proportional to the wave number: $\omega = v_0\xi$; so that, from (11.32) and (11.35),

$$\theta_{AC} = (d_{74} - j_{17}e_{14})e_{14}\rho\omega^2/(c^E_{44})^2. \tag{11.36}$$

Thus, at frequencies up to, say, 10^{10} cps, the acoustical rotatory power is approximately proportional to the square of the frequency and depends on the constants ρ, e_{14} and c^E_{44}, which are commonly encountered in piezoelectricity theory, and also on the constants d_{74} and j_{17}, which control the coupling of the polarization gradient with the strain and polarization, respectively.

For α-quartz, all the quantities in the formula (11.29) for optical rotatory power are known except j_{17}. Thus, for left-handed quartz and the sodium D line,

$$\begin{aligned} \theta_{OP} &= -379 \text{ radian/meter} && [61, \text{p.}481], \\ \lambda_0 &= 5893 \times 10^{-10} \text{ meter} && [61, \text{p.}481], \\ n &= 1.5533 && [61, \text{p.}481], \\ \epsilon_0 &= 8.854 \times 10^{-12} \text{ farad/meter} && [60]. \end{aligned}$$

Hence,

$$j_{17} = -\theta_{OP}\lambda_0^2/4\pi^2\epsilon_0(n^2-1)^2 = 0.19 \text{ meter}^2/\text{farad}. \tag{11.37}$$

With the value of j_{17} known, all quantities in the formula (11.36) for acoustical rotatory power are known except d_{74}. In particular, Pine [56] finds that the acoustical and optical activities have opposite signs and the acoustical rotatory power along the trigonal axis is about 220 radians/meter at one gigahertz. Thus, for lefthanded α-quartz,

$\theta_{AC} = 220$ radian/meter [56],

$\omega = 2\pi \times 10^9$ radian/second [56],

$\rho = 2.65 \times 10^3$ kilogram/meter^3 [62],

$c_{44}^E = 57.94 \times 10^9$ newton/meter^2 [63],

$e_{14} = -0.0406$ coulomb/meter^2 [65].

Hence,

$$d_{74} = \theta_{AC}(c_{44}^E)^2/e_{14}\rho\omega^2 + j_{17}e_{14} = -174 - 0.0077 \text{ volt.} \qquad (II.38)$$

The second term, $j_{17}e_{14}$, is negligible in comparison with the first, so that we may drop the dependence of acoustical rotatory power on j_{17}, i.e. on the interaction between polarization and polarization gradient, and replace (II.36) with

$$\theta_{AC} = d_{74}e_{14}\rho\omega^2/(c_{44}^E)^2. \qquad (II.39)$$

Thus, according to this theory, the presence of acoustical activity in α-quartz depends on the existence of the piezoelectric stress constant e_{14}, $= e_{123}$, and the interaction constant d_{74}, $= d_{3223}$, between strain and polarization; whereas the presence of optical activity depends only on the existence of the interaction constant j_{17}, $= j_{132}$, between polarization and polarization gradient.

12. Diatomic, Elastic, Dielectric Continuum and Lattice

i. Potential and Kinetic Energies.

A continuum theory of a crystal with two polarizable atoms per cell may be produced by combining the procedures employed in Articles 4 and 7 [64]. Atoms in the two component continua are again identified by 1 and 2 with displacements now designated by $u_i^{(\kappa)}$, κ 1,2, and polarizations by $P_i^{(\kappa)}$, as illustrated in Fig. 17; while polarization gradients, strains, relative displacement and relative rotation are denoted by

$$P_{j,i}\ ,\quad S_{ij}^{(\kappa)}=\tfrac{1}{2}\left(u_{j,i}^{(\kappa)}+u_{i,j}^{(\kappa)}\right)\ ,\quad u_i^{*}=u_i^{(2)}-u_i^{(1)}\ ,\quad \omega_{ij}^{*}=\tfrac{1}{2}\left(u_{j,i}^{*}-u_{i,j}^{*}\right), \tag{12.1}$$

respectively. The potential energy density of deformation and polarization is assumed to be a quadratic function of $S_{ij}^{(\kappa)}$, $P_i^{(\kappa)}$, $P_{j,i}^{(\kappa)}$, u_i^{*} and ω_{ij}^{*} :

$$W^{L}=W^{L}\left(S_{ij}^{(1)},\ S_{ij}^{(2)},\ P_i^{(1)},\ P_i^{(2)},\ P_{j,i}^{(1)},\ P_{j,i}^{(2)},\ u_i^{*},\ \omega_{ij}^{*}\right). \tag{12.2}$$

The total potential energy density, W, is again the energy density of deformation and polarization augmented by the energy density of the Maxwell, electric self-field $E_i=-\varphi_{,i}$:

$$W=W^{L}+\tfrac{1}{2}\epsilon_0\varphi_{,i}\varphi_{,i}\,. \tag{12.3}$$

The associated kinetic energy density is, again,

$$T=\sum_{\kappa}\tfrac{1}{2}\rho^{(\kappa)}\dot{u}_i^{(\kappa)}\dot{u}_i^{(\kappa)}\ ,\quad \kappa=1,2\,;\ \ i=1,2,3, \tag{12.4}$$

where $\rho^{(1)}$ and $\rho^{(2)}$ are the mass densities of the two continua and the "over-dot" notation designates differentiation with respect to time.

ii. Field Equations and Boundary Conditions.

The field equations and boundary conditions, corresponding to the potential and kinetic energy densities (12.3) and (12.4), may be derived, as in Article 7, by means of an extension of a linear version

of Toupin's [42] variational principle for the classical theory of elastic dielectrics. The extension accounts for the contributions of the polarization gradient, the two continua and the kinetic energy.

First, we define an electric enthalpy density — the energy density diminished by the product of the Maxwell self-field, E_i, and the electric displacement D_i:

$$H = W - E_i D_i , \tag{12.5}$$

where

$$D_i = \epsilon_0 E_i + P_i , \tag{12.6}$$

$$E_i = -\varphi_{,i} , \tag{12.7}$$

$$P_i = P_i^{(1)} + P_i^{(2)} + q_* u_i^* . \tag{12.8}$$

The inclusion of the term $q_* u_i^*$, in the polarization density P_i, was suggested by P.C.Y. Lee to accommodate applications to ionic crystals. The product of the charge density q_* and the relative displacement u_i^* represents the ionic, or atomic, polarization as distinguished from the electronic polarizations $P_i^{(k)}$. In what follows, if q_* is not set equal to zero, the superscript $k=1$ identifies the positive ion and $k=2$ the negative ion.

Inserting (12.3) and (12.6)-(12.8) in (12.5), we find

$$H = W^L - \tfrac{1}{2}\epsilon_0 \varphi_{,i}\varphi_{,i} + \varphi_{,i}\left(P_i^{(1)} + P_i^{(2)} + q_* u_i^*\right). \tag{12.9}$$

In a body occupying a volume V bounded by a surface S separating V from a vacuum V', the extension of Toupin's variational principle takes the form

$$\delta\int_{t_0}^{t_1} dt \int_{V^*} (T-H)\,dV + \sum_k \int_{t_0}^{t_1} dt \int_V \left(f_i^{(k)}\delta u_i^{(k)} + E_i^{\circ}\delta P_i^{(k)} + E_i^{(o)} q_* \delta u_i^*\right) dV$$
$$+ \sum_k \int_{t_0}^{t_1} dt \int_S t_i^{(k)} \delta u_i^{(k)}\, dS = 0, \quad k=1,2, \tag{12.10}$$

for independent variations of $u_i^{(k)}$, $P_i^{(k)}$ and φ between fixed limits at times t_0 and t_1. In (12.10), $V^* = V + V'$, $f_i^{(k)}$ and $t_i^{(k)}$ are the external body forces

and surface tractions on the two continua and E_i° is the external electric field. Now,

$$\delta W^L = \sum_\kappa \left(T_{ij}^{(\kappa)} \delta S_{ij}^{(\kappa)} - E_i^{(\kappa)} \delta P_i^{(\kappa)} + E_{ij}^{(\kappa)} \delta P_{j,i}^{(\kappa)} \right) + T_i^* \delta u_i^* + T_{ij}^* \delta \omega_{ij}^* , \qquad (12.11)$$

where

$$T_{ij}^{(\kappa)} = \frac{\partial W^L}{\partial S_{ij}^{(\kappa)}} , \quad E_i^{(\kappa)} = -\frac{\partial W^L}{\partial P_i^{(\kappa)}} , \quad E_{ij}^{(\kappa)} = \frac{\partial W^L}{\partial P_{j,i}^{(\kappa)}} , \quad T_i^* = \frac{\partial W^L}{\partial u_i^*} , \quad T_{ij}^* = \frac{\partial W^L}{\partial \omega_{ij}^*} . \qquad (12.12)$$

Note that the $E_i^{(\kappa)}$ are the effective local fields of the two continua: as distinguished from the Maxwell self-field E_i.

With the chain rule of differentiation, (12.11) becomes

$$\delta W^L = -\sum_\kappa \left[T_{ij,i}^{(\kappa)} + (-1)^\kappa \left(T_{ij,i}^* - T_j^* \right) \right] \delta u_j^{(\kappa)} - \sum_\kappa \left(E_j^{(\kappa)} + E_{ij,i}^{(\kappa)} \right) \delta P_j^{(\kappa)}$$

$$+ \sum_\kappa \left\{ \left[T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^* \right] \delta u_j^{(\kappa)} \right\}_{,i} + \sum_\kappa \left(E_{ij}^{(\kappa)} \delta P_j^{(\kappa)} \right)_{,i} .$$

Treating the remaining part of H in (12.9) similarly, we have, in V:

$$\delta H = -\sum_\kappa \left[T_{ij,i}^{(\kappa)} + (-1)^\kappa \left(T_{ij,i}^* - T_j^* - q_* \varphi_{,i} \right) \right] \delta u_j^{(\kappa)} - \sum_\kappa \left(E_j^{(\kappa)} + E_{ij,i}^{(\kappa)} - \varphi_{,i} \right) \delta P_j^{(\kappa)}$$

$$+ \sum_\kappa \left[\epsilon_0 \varphi_{,ii} - P_{i,i}^{(\kappa)} - (-1)^\kappa q_* u_{i,i}^{(\kappa)} \right] \delta\varphi + \sum_\kappa \left\{ \left[T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^* \right] \delta u_j^{(\kappa)} \right\}_{,i}$$

$$+ \sum_\kappa \left(E_{ij}^{(\kappa)} \delta P_j^{(\kappa)} \right)_{,i} - \sum_\kappa \left\{ \left[\epsilon_0 \varphi_{,i} - P_i^{(\kappa)} - (-1)^\kappa q_* u_i^{(\kappa)} \right] \delta\varphi \right\}_{,i} ; \qquad (12.13)$$

and, in V':

$$\delta H = \epsilon_0 \varphi_{,ii} \delta\varphi - \epsilon_0 \left(\varphi_{,i} \delta\varphi \right)_{,i} . \qquad (12.14)$$

Further, from (12.4),

$$\delta \int_{t_0}^{t_1} T\, dt = -\sum_\kappa \int_{t_0}^{t_1} \rho^{(\kappa)} \ddot{u}_i^{(\kappa)} \delta u_i^{(\kappa)} dt . \qquad (12.15)$$

Inserting (12.13)-(12.15) in (12.10) and applying the divergence theorem where appropriate, we find

$$\sum_\kappa \int_{t_0}^{t_1} dt \int_V \left[T_{ij,i}^{(\kappa)} + (-1)^\kappa \left(T_{ij,i}^* - T_j^* - q_* \varphi_{,j} \right) + (-1)^\kappa q_* E_j^\circ + f_j^{(\kappa)} - \rho^{(\kappa)} \ddot{u}_j^{(\kappa)} \right] \delta u_j^{(\kappa)} dV$$

$$+ \sum_\kappa \int_{t_0}^{t_1} dt \int_V \left\{ \left(E_j^{(\kappa)} + E_{ij,i}^{(\kappa)} - \varphi_{,j} + E_j^\circ \right) \delta P_j^{(\kappa)} + \left[-\epsilon_0 \varphi_{,ii} + P_{i,i}^{(\kappa)} + (-1)^\kappa q_* u_{i,i}^{(\kappa)} \right] \delta\varphi \right\} dV$$

$$- \sum_{K} \int_{t_0}^{t_1} dt \int_S \{ n_i [T_{ij}^{(K)} + (-1)^K T_{ij}^*] - t_j^{(K)} \} \delta u_j^{(K)} \, dS$$

$$- \sum_{K} \int_{t_0}^{t_1} dt \int_S \{ n_i E_{ij}^{(K)} \delta P_j^{(K)} + n_i [-\epsilon_0 [\varphi_{,i}] + P_i^{(K)} + q_* (-1)^K u_i^{(K)}] \delta\varphi \, dS$$

$$- \int_{t_0}^{t_1} dt \int_{V'} \epsilon_0 \varphi_{,ii} \, \delta\varphi \, dV = 0. \qquad (12.16)$$

where n_i is the unit outward normal to S and $[\varphi_{,i}]$ is the jump in $\varphi_{,i}$ across S.

From (12.16), we have the Euler equations in V:

$$\begin{aligned} T_{ij,i}^{(K)} + (-1)^K (T_{ij,i}^* - T_j^* - q_* \varphi_{,i}) + f_j^{(K)} + (-1)^K q_* E_j^\circ &= \rho^{(K)} \ddot{u}_j^{(K)}, \\ E_j^{(K)} + E_{ij,i}^{(K)} - \varphi_{,j} + E_j^\circ &= 0, \\ -\epsilon_0 \varphi_{,ii} + P_{i,i}^{(1)} + P_{i,i}^{(2)} + q_* u_{i,i}^* &= 0; \end{aligned} \qquad (12.17)$$

and, in V':

$$\varphi_{,ii} = 0; \qquad (12.18)$$

and also the boundary conditions on S:

$$\begin{aligned} n_i [T_{ij}^{(K)} + (-1)^K T_{ij}^*] &= t_j^{(K)}, \\ n_i E_{ij}^{(K)} &= 0, \\ n_i (-\epsilon_0 [\varphi_{,i}] + P_i^{(1)} + P_i^{(2)} + q_* u_i^*) &= 0. \end{aligned} \qquad (12.19)$$

As may be seen from (12.16), boundary conditions alternative to each of (12.19) are the specification of $u_i^{(K)}$, $P_i^{(K)}$ and φ, respectively.

iii Constitutive Equations.

We consider the constitutive equations for a crystal with NaCl-type lattice structure, which falls under cubic point group m3m, the generators for which are given in (7.10). Owing to the first generator in (7.10) (the centro-symmetry generator) there can be no coefficients of odd rank and no products of symmetric and antisymmetric variables in the quadratic function W^L. This reduces the interactions to those between variables connected by full lines in Fig. 18; whereas the dashed line segments denote excluded interactions. The corresponding energy function is

$$W^L = \frac{1}{2}\sum_{\kappa,\lambda}\left(a_{ij}^{\kappa\lambda}P_i^{(\kappa)}P_j^{(\lambda)} + b_{ijk\ell}^{\kappa\lambda}P_{j,i}^{(\kappa)}P_{\ell,k}^{(\lambda)} + c_{ijk\ell}^{\kappa\lambda}S_{ij}^{(\kappa)}S_{k\ell}^{(\lambda)} + 2d_{ijk\ell}^{\kappa\lambda}P_{(j,i)}^{(\kappa)}S_{k\ell}^{(\lambda)}\right)$$
$$+\sum_{\kappa}\left(a^{*\kappa}u_i^*P_i^{(\kappa)} + 2d^{*\kappa}\omega_{ij}^*P_{[j,i]}^{(\kappa)}\right) + \frac{1}{2}a^{**}u_i^*u_i^* + c^{**}\omega_{ij}^*\omega_{ij}^*$$
$$+\sum_{\kappa}\left(b^{\kappa 0}P_{i,i}^{(\kappa)} + c^{\kappa 0}S_{ii}^{(\kappa)}\right), \qquad (12.20)$$

where $P_{(j,i)}^{(\kappa)}$ and $P_{[j,i]}^{(\kappa)}$ denote the symmetric and antisymmetric parts of $P_{j,i}^{(\kappa)}$, respectively. We note that, in general,

$$a_{ij}^{\kappa\lambda} = a_{ij}^{\lambda\kappa}, \quad b_{ijk\ell}^{\kappa\lambda} = b_{ijk\ell}^{\lambda\kappa}, \quad c_{ijk\ell}^{\kappa\lambda} = c_{ijk\ell}^{\lambda\kappa}, \quad d_{ijk\ell}^{\kappa\lambda} \neq d_{ijk\ell}^{\lambda\kappa} \qquad (12.21)$$

and, from (7.10),

$$\begin{aligned}
a_{ij}^{\kappa\lambda} &= a_{11}^{\kappa\lambda}\delta_{ij},\\
b_{ijk\ell}^{\kappa\lambda} &= b^{\kappa\lambda}\delta_{ijk\ell} + b_{12}^{\kappa\lambda}\delta_{ij}\delta_{k\ell} + b_{44}^{\kappa\lambda}(\delta_{ik}\delta_{j\ell}+\delta_{i\ell}\delta_{jk}) + b_{77}^{\kappa\lambda}(\delta_{ik}\delta_{j\ell}-\delta_{i\ell}\delta_{jk}),\\
c_{ijk\ell}^{\kappa\lambda} &= c^{\kappa\lambda}\delta_{ijk\ell} + c_{12}^{\kappa\lambda}\delta_{ij}\delta_{k\ell} + c_{44}^{\kappa\lambda}(\delta_{ik}\delta_{j\ell}+\delta_{i\ell}\delta_{jk}),\\
d_{ijk\ell}^{\kappa\lambda} &= d^{\kappa\lambda}\delta_{ijk\ell} + d_{12}^{\kappa\lambda}\delta_{ij}\delta_{k\ell} + d_{44}^{\kappa\lambda}(\delta_{ik}\delta_{j\ell}+\delta_{i\ell}\delta_{jk}),
\end{aligned} \qquad (12.22)$$

where δ_{ij} (or $\delta_{ijk\ell}$) is unity when its indices are alike and zero otherwise;

$$b^{\kappa\lambda} = b_{11}^{\kappa\lambda} - b_{12}^{\kappa\lambda} - 2b_{44}^{\kappa\lambda}, \quad c^{\kappa\lambda} = c_{11}^{\kappa\lambda} - c_{12}^{\kappa\lambda} - 2c_{44}^{\kappa\lambda}, \quad d^{\kappa\lambda} = d_{11}^{\kappa\lambda} - c_{12}^{\kappa\lambda} - 2d_{44}^{\kappa\lambda}; \qquad (12.23)$$

for $b_{ijk\ell}^{\kappa\lambda}$, $c_{ijk\ell}^{\kappa\lambda}$ and $d_{ijk\ell}^{\kappa\lambda}$, the abbreviated notation for pairs of indices, ij or $k\ell$, has been used — as in Article 11. It may be observed that material constants with superscripts 11 or 22 denote interactions within one of the two component continua whereas constants with superscripts 12 or 21 denote interactions between the two component continua.

From (12.12) and (12.20) - (12.22), we find the constitutive equations

$$\begin{aligned}
T_{ij}^{(\kappa)} &= c^{\kappa 0}\delta_{ij} + \sum_{\lambda}\left(c^{\kappa\lambda}\delta_{ijk\ell}S_{k\ell}^{(\lambda)} + c_{12}^{\kappa\lambda}\delta_{ij}S_{kk}^{(\lambda)} + 2c_{44}S_{ij}^{(\lambda)}\right) + \sum_{\lambda}\left(d^{\lambda\kappa}\delta_{ijk\ell}P_{\ell,k}^{(\lambda)} + d_{12}^{\lambda\kappa}\delta_{ij}P_{k,k}^{(\lambda)} + 2d_{44}^{\lambda\kappa}P_{(j,i)}^{(\lambda)}\right),\\
-E_j^{(\kappa)} &= \sum_{\lambda}a_{11}^{\kappa\lambda}P_j^{(\lambda)} + a^{*\kappa}u_j^*,\\
E_{ij}^{(\kappa)} &= b^{\kappa 0}\delta_{ij} + \sum_{\lambda}\left(b^{\kappa\lambda}\delta_{ijk\ell}P_{\ell,k}^{(\lambda)} + b_{12}^{\kappa\lambda}\delta_{ij}P_{k,k}^{(\lambda)} + 2b_{44}^{\kappa\lambda}P_{(j,i)}^{(\lambda)} + 2b_{77}^{\kappa\lambda}P_{[j,i]}^{(\lambda)}\right)\\
&\quad + 2d^{*\kappa}\omega_{ij}^* + \sum_{\lambda}\left(d^{\kappa\lambda}\delta_{ijk\ell}S_{k\ell}^{(\lambda)} + d_{12}^{\kappa\lambda}\delta_{ij}S_{kk}^{(\lambda)} + 2d_{44}^{\kappa\lambda}S_{ij}^{(\lambda)}\right),\\
T_j^* &= \sum_{\lambda}a^{*\lambda}P_j^{(\lambda)} + a^{**}u_j^*,\\
T_{ij}^* &= 2\sum_{\lambda}d^{*\lambda}P_{[j,i]}^{(\lambda)} + 2c^{**}\omega_{ij}^*.
\end{aligned} \qquad (12.24)$$

We shall assume that, in the initial state, i.e. when

$$P_i^{(\kappa)},\ P_{j,i}^{(\kappa)},\ S_{ij}^{(\kappa)},\ u_i^*,\ \omega_{ij}^*,\ \varphi_{,i},\ f_i^{(\kappa)},\ E_i^\circ = 0,$$

there is no resultant force across any surface — exterior or interior. That is

$$t_i^{(1)} + t_j^{(2)} = 0.$$

Then, from the first of (12.19),

$$n_i T_{ij}^{(1)} + n_i T_{ij}^{(2)} = 0;$$

so that, from the first of (12.24),

$$c^{10} + c^{20} = 0. \qquad (12.25)$$

Accordingly, from (12.22) and (12.25), in the initial state:

$$E_i^{(\kappa)},\ T_i^*,\ T_{ij}^* = 0, \quad T_{ij}^{(1)} + T_{ij}^{(2)} = 0,$$

but there is a self-equilibrated

$$E_{ij}^{(\kappa)} = b^{\kappa 0}\delta_{ij}$$

in each component continuum.

iv. Surface Energy of Deformation and Polarization.

In a state of equilibrium, the total energy in V^* is, from (12.3),

$$\mathcal{W} = \int_V W^L dV + \frac{1}{2}\int_{V^*} \epsilon_0 \varphi_{,i}\varphi_{,i}\, dV. \qquad (12.26)$$

We can write W^L in the form

$$2W^L = \sum_\kappa \left(T_{ij}^{(\kappa)} S_{ij}^{(\kappa)} - E_i^{(\kappa)} P_i^{(\kappa)} + E_{ij}^{(\kappa)} P_{j,i}^{(\kappa)}\right) + T_i^* u_i^* + T_{ij}^* \omega_{ij}^* + \sum_\kappa b^{\kappa 0} P_{i,i}^{(\kappa)} + c^{20}\left(S_{ii}^{(2)} - S_{ii}^{(1)}\right).$$

Then, by the same procedure as that employed in arriving at (12.16),

$$\int_V W^L dV = -\frac{1}{2}\sum_\kappa \int_V \{[T_{ij,i}^{(\kappa)} + (-1)^\kappa (T_{ij,i}^* - T_j^*)]u_j^{(\kappa)} + (E_j^{(\kappa)} + E_{ij,i}^{(\kappa)})P_j^{(\kappa)}\}dV$$
$$+ \frac{1}{2}\sum_\kappa \int_S n_i\{[T_{ij}^{(\kappa)} + (-1)^\kappa T_{ij}^*]u_j^{(\kappa)} + E_{ij}^{(\kappa)} P_j^{(\kappa)}\}dS + \frac{1}{2}\sum_\kappa \int_S n_i (b^{\kappa 0} P_i^{(\kappa)} + c^{\kappa 0} u_i^*)dS. \qquad (12.27)$$

Also,

$$\int_{V^*} \varphi_{,i}\varphi_{,i}\,dV = -\int_{V^*} \varphi_{,ii}\varphi\,dV + \int_S n_i [\varphi_{,i}]\varphi\,dS. \qquad (12.28)$$

Inserting (12.27) and (12.28) in (12.26) and applying the equations of equilibrium, i.e. (12.17) with $u^{(k)}_{j,tt} = 0$, in the absence of external forces ($f^{(k)}, E^\circ_j = 0$) we find

$$2W = -\sum_k \int_V [(-1)^k q_* \varphi_{,i} u_i^{(k)} + \varphi_{,i} P_i^{(k)} + (P^{(k)}_{i,i} + q_* u^*_{i,i})\varphi]\,dV$$
$$+ \sum_k \int_S n_i\{[T^{(k)}_{ij} + (-1)^k T^*_{ij}]u^{(k)}_j + E^{(k)}_{ij} P^{(k)}_j + \epsilon_0 [\varphi_{,i}]\varphi\}dS + \sum_k \int_S n_i (b^{k0} P^{(k)}_i + c^{20} u^*_i) dS.$$

Now

$$\int_V P^{(k)}_{i,i}\varphi\,dV = -\int_V \varphi_{,i} P^{(k)}_i\,dV + \int_S n_i P^{(k)}\varphi\,dS,$$

$$\int_V q_* (u^*_i \varphi_{,i} + u^*_{i,i}\varphi)\,dV = \int_S n_i q_* u^*_i \varphi\,dS.$$

Hence

$$2W = \sum_k \int_S n_i\{[T^{(k)}_{ij} + (-1)^k T^*_{ij}]u^{(k)}_j + E^{(k)}_{ij} P^{(k)}_j + (\epsilon_0[\varphi_{,i}] - P^{(k)}_i - q_* u^*_i)\varphi\}dS$$
$$+ \sum_k \int_S n_i (b^{k0} P^{(k)}_i + c^{20} u^*_i) dS. \qquad (12.29)$$

From (12.19) the first integral in (12.29) vanishes if the boundary is entirely free. In that case,

$$2W = \sum_k \int_S n_i (b^{k0} P^{(k)}_i + c^{20} u^*_i)\,dS.$$

Accordingly, the surface energy of deformation and polarization, per unit area, is

$$W^S = \tfrac{1}{2} n_i [b^{10} P^{(1)}_i + b^{20} P^{(2)}_i + c^{20} u^*_i]_S. \qquad (12.30)$$

This result is to be compared with (10.9).

v. Wave Motion.

The equations of motion in terms of $u^{(k)}_i$, $P^{(k)}_i$ and φ are obtained by substituting the constitutive equations (12.24) into the field equations (12.17) with the result, for each k,

$$\sum_{\lambda}[c^{\kappa\lambda}\delta_{ijk\ell}u^{(\lambda)}_{\ell,ki}+c^{\kappa\lambda}_{12}u^{(\lambda)}_{i,ij}+c^{\kappa\lambda}_{44}(u^{(\lambda)}_{j,ii}+u^{(\lambda)}_{i,ij})]$$
$$+\sum_{\lambda}[d^{\lambda\kappa}\delta_{ijk\ell}P^{(\lambda)}_{\ell,ki}+d^{\lambda\kappa}_{12}P^{(\lambda)}_{i,ij}+d^{\lambda\kappa}_{44}(P^{(\lambda)}_{j,ii}+P^{(\lambda)}_{i,ij})]$$
$$+(-1)^{\kappa}\sum_{\lambda}[d^{*\lambda}(P^{(\lambda)}_{j,ii}-P^{(\lambda)}_{i,ij})+(-1)^{\lambda}c^{**}(u^{(\lambda)}_{j,ii}-u^{(\lambda)}_{i,ij})]$$
$$-(-1)^{\kappa}[a^{*1}P^{(1)}_j+a^{*2}P^{(2)}_j+a^{**}(u^{(2)}_j-u^{(1)}_j)+q_*\varphi_{,j}-q_*E^{\circ}_j+f^{(\kappa)}_j=\rho^{(\kappa)}\ddot{u}^{(\kappa)}_j\ ,$$

$$\sum_{\lambda}[d^{\kappa\lambda}\delta_{ijk\ell}u^{(\lambda)}_{\ell,ki}+d^{\kappa\lambda}_{12}u^{(\lambda)}_{i,ij}+d^{\kappa\lambda}_{44}(u^{(\lambda)}_{j,ii}+u^{(\lambda)}_{i,ij})+(-1)^{\lambda}d^{*\kappa}(u^{(\lambda)}_{j,ii}-u^{(\lambda)}_{i,ij})]$$
$$+\sum_{\lambda}[b^{\kappa\lambda}\delta_{ijk\ell}P^{(\lambda)}_{\ell,ki}+b^{\kappa\lambda}_{12}P^{(\lambda)}_{i,ij}+b^{\kappa\lambda}_{44}(P^{(\lambda)}_{j,ii}+P^{(\lambda)}_{i,ij})+b^{\kappa\lambda}_{77}(P^{(\lambda)}_{j,ii}-P^{(\lambda)}_{i,ij})]$$
$$a^{1\kappa}_{11}P^{(1)}_j-a^{2\kappa}_{11}P^{(2)}_j-a^{*\kappa}(u^{(2)}_j-u^{(1)}_j)-\varphi_{,j}+E^{\circ}_j=0, \tag{12.31}$$

$$-\epsilon_0\varphi_{,ii}+P^{(1)}_{i,i}+P^{(2)}_{i,i}+q_*(u^{(2)}_{i,i}-u^{(1)}_{i,i})=0.$$

The essential features of wave motion are revealed by an examination of plane waves in, say, the x_1, or (100), direction:

$$u^{(\kappa)}_j=A^{(\kappa)}_je^{i(\xi x_1-\omega t)},\quad P^{(\kappa)}_j=B^{(\kappa)}_je^{i(\xi x_1-\omega t)},\quad \varphi=Ce^{i(\xi x_1-\omega t)} \tag{12.32}$$

and $f^{(\kappa)}_j, E^{\circ}_j=0$. With these functions, the five equations (12.31) reduce to those for longitudinal waves if $j=1$ and transverse waves if $j=2$ or 3. Thus:

Longitudinal $(j=1)$

$$c^{11}_{11}u^{(1)}_{1,11}+c^{12}_{11}u^{(2)}_{1,11}+d^{11}_{11}P^{(1)}_{1,11}+d^{21}_{11}P^{(2)}_{1,11}+a^{*1}P^{(1)}_1+a^{*2}P^{(2)}_1+a^{**}(u^{(2)}_1-u^{(1)}_1)+q_*\varphi_{,1}=\rho^{(1)}\ddot{u}^{(1)}_1\ ,$$
$$c^{21}_{11}u^{(1)}_{1,11}+c^{22}_{11}u^{(2)}_{1,11}+d^{12}_{11}P^{(1)}_{1,11}+d^{22}_{11}P^{(2)}_{1,11}-a^{*1}P^{(1)}_1-a^{*2}P^{(2)}_1-a^{**}(u^{(2)}_1-u^{(1)}_1)-q_*\varphi_{,1}=\rho^{(2)}\ddot{u}^{(2)}_1\ ,$$
$$d^{11}_{11}u^{(1)}_{1,11}+d^{12}_{11}u^{(2)}_{1,11}+b^{11}_{11}P^{(1)}_{1,11}+b^{12}_{11}P^{(2)}_{1,11}-a^{11}_{11}P^{(1)}_1-a^{12}_{11}P^{(2)}_1-a^{*1}(u^{(2)}_1-u^{(1)}_1)-\varphi_{,1}=0, \tag{12.33}$$
$$d^{21}_{11}u^{(1)}_{1,11}+d^{22}_{11}u^{(2)}_{1,11}+b^{21}_{11}P^{(1)}_{1,11}+b^{22}_{11}P^{(2)}_{1,11}-a^{21}_{11}P^{(1)}_1-a^{22}_{11}P^{(2)}_1-a^{*2}(u^{(2)}_1-u^{(1)}_1)-\varphi_{,1}=0,$$
$$P^{(1)}_{1,1}+P^{(2)}_{1,1}+q_*(u^{(2)}_{1,1}-u^{(1)}_{1,1})-\epsilon_0\varphi_{,11}=0.$$

Transverse $(j=2)$

$$(c^{11}_{44}-c^{**})u^{(1)}_{2,11}+(c^{12}_{44}+c^{**})u^{(2)}_{2,11}+(d^{11}_{44}-d^{*1})P^{(1)}_{2,11}+(d^{21}_{44}-d^{*2})P^{(2)}_{2,11}$$
$$+a^{*1}P^{(1)}_2+a^{*2}P^{(2)}_2+a^{**}(u^{(2)}_2-u^{(1)}_2)=\rho^{(1)}\ddot{u}^{(1)}_2\ ,$$
$$(c^{21}_{44}+c^{**})u^{(1)}_{2,11}+(c^{22}_{44}-c^{**})u^{(2)}_{2,11}+(d^{12}_{44}+d^{*1})P^{(1)}_{2,11}+(d^{22}_{44}+d^{*2})P^{(2)}_{2,11}$$
$$-a^{*1}P^{(1)}_2-a^{*2}P^{(2)}_2-a^{**}(u^{(2)}_2-u^{(1)}_2)=\rho^{(2)}\ddot{u}^{(2)}_2\ , \tag{12.34}$$
$$(d^{11}_{44}-d^{*1})u^{(1)}_{2,11}+(d^{12}_{44}+d^{*1})u^{(2)}_{2,11}+(b^{11}_{44}+b^{11}_{77})P^{(1)}_{2,11}+(b^{12}_{44}+b^{12}_{77})P^{(2)}_{2,11}$$
$$-a^{11}_{11}P^{(1)}_2-a^{12}_{11}P^{(2)}_2-a^{*1}(u^{(2)}_2-u^{(1)}_2)=0,$$

$$(d_{44}^{21} - a^{*2})u_{2,11}^{(1)} + (d_{44}^{22} + a^{*2})u_{2,11}^{(2)} + (b_{44}^{21} + b_{77}^{21})P_{2,11}^{(1)} + (b_{44}^{22} + b_{77}^{22})P_{2,11}^{(2)}$$
$$- a_{11}^{21}P_2^{(1)} - a_{11}^{22}P_2^{(2)} - a^{*2}(u_2^{(2)} - u_2^{(1)}) = 0.$$

It may be noted that the Maxwell self-field is coupled to the mechanical displacement in the longitudinal waves, but not in the transverse waves. As is shown in the following Article, if the magnetic field is taken into account, the longitudinal wave is unchanged but there is full coupling of the elastic and electromagnetic fields in the transverse wave.

Upon substituting (12.32) in (12.33) and eliminating $A_i^{(\kappa)}$, $B_i^{(\kappa)}$ and C_i we find the dispersion relation for longitudinal waves:

$$\Delta_L = 0, \tag{12.35}$$

where Δ_L is the determinant with elements

$$\begin{aligned}
\Delta_{11} &= \rho^{(1)}\omega^2 - a^{**} - q_*^2\epsilon_0^{-1} - c_{11}^{11}\xi^2, & \Delta_{23} &= -a^{*1} - q_*\epsilon_0^{-1} - d_{11}^{12}\xi^2 = \Delta_{32},\\
\Delta_{12} &= a^{**} + q_*^2\epsilon_0^{-1} - c_{11}^{12}\xi^2 = \Delta_{21}, & \Delta_{24} &= -a^{*2} - q_*\epsilon_0^{-1} - d_{11}^{22}\xi^2 = \Delta_{42},\\
\Delta_{13} &= a^{*1} + q_*\epsilon_0^{-1} - d_{11}^{11}\xi^2 = \Delta_{31}, & \Delta_{33} &= -a_{11}^{11} - \epsilon_0^{-1} - b_{11}^{11}\xi^2,\\
\Delta_{14} &= a^{*2} + q_*\epsilon_0^{-1} - d_{11}^{21}\xi^2 = \Delta_{41}, & \Delta_{34} &= -a_{11}^{21} - \epsilon_0^{-1} - b_{11}^{21}\xi^2 = \Delta_{43},\\
\Delta_{22} &= \rho^{(2)}\omega^2 - a^{**} - q_*^2\epsilon_0^{-1} - c_{11}^{11}\xi^2, & \Delta_{44} &= -a_{11}^{22} - \epsilon_0^{-1} - b_{11}^{22}\xi^2.
\end{aligned} \tag{12.36}$$

This is a quartic equation in ξ^2. Of the four branches, two are real: one acoustical and one optical, as may be verified by showing that one real branch passes through $\xi = 0$, $\omega = 0$ and one through $\xi = 0$, $\omega \neq 0$. We find, in fact,

$$\lim_{\omega,\xi\to 0} \Delta_L = \lim_{\omega,\xi\to 0} \left[(c_{11}^{11} + c_{11}^{22} + 2c_{11}^{12})\xi^2 - (\rho^{(1)} + \rho^{(2)})\omega^2 \right] D_L, \tag{12.37}$$

where

$$D_L = \begin{vmatrix} a_{11}^{11} + \epsilon_0^{-1} & a_{11}^{12} + \epsilon_0^{-1} & a^{*1} + q_*\epsilon_0^{-1} \\ a_{11}^{21} + \epsilon_0^{-1} & a_{11}^{22} + \epsilon_0 & a^{*2} + q_*\epsilon_0^{-1} \\ a^{*1} + q_*\epsilon_0^{-1} & a^{*2} + q_*\epsilon_0^{-1} & a^{**} + q_*^2\epsilon_0^{-1} \end{vmatrix}. \tag{12.38}$$

Hence, at long wave lengths, the frequency of the longitudinal acoustic wave is

$$\omega_{LA} = \xi\left[\left(c_{11}^{11} + c_{11}^{22} + 2c_{11}^{12}\right)/\left(\rho^{(1)} + \rho^{(2)}\right)\right]^{1/2}. \tag{12.39}$$

It may be seen, from (12,39), that the usual low frequency extensional stiffness, c_{11}, is given by

$$c_{11} = c_{11}^{11} + c_{11}^{22} + 2c_{11}^{12}, \tag{12.40}$$

i.e. the sum of the extensional stiffnesses, c_{11}^{11} and c_{11}^{22}, of the two component continua augmented by the intercomponent extensional stiffness $2c_{11}^{12}$.

The long wave limit of the longitudinal optical branch is obtained from

$$\lim_{\xi\to 0} \Delta_L = \omega^2\left\{\rho^{(1)}\rho^{(2)}\omega^2\left[\left(a_{11}^{11} + \epsilon_0^{-1}\right)\left(a_{11}^{22} + \epsilon_0^{-1}\right) - \left(a_{11}^{12} + \epsilon_0^{-1}\right)^2\right] - \left(\rho^{(1)} + \rho^{(2)}\right)D_L\right\}, \tag{12.41}$$

Hence, the limiting frequency of the longitudinal optical brach is

$$\omega_{LO} = \left\{D_L\epsilon_0^2/\bar{\rho}\left[\left(1 + a_{11}^{11}\epsilon_0\right)\left(1 + a_{11}^{22}\epsilon_0\right) - \left(1 + a_{11}^{12}\epsilon_0\right)^2\right\}^{1/2}, \tag{12.42}$$

where

$$\bar{\rho} = \rho^{(1)}\rho^{(2)}/\left(\rho^{(1)} + \rho^{(2)}\right), \tag{12.43}$$

i.e. $\bar{\rho}$ is the reduced density.

In a similar way, we find, from (12.34), the dispersion relation for transverse waves in the (100) direction:

$$\Delta_T = 0, \tag{12.44}$$

where Δ_T is the determinant with elements

$$\begin{aligned}
\Delta_{11} &= \rho^{(1)}\omega^2 - a^{**} - \left(c_{44}^{11} - c^{**}\right)\xi^2, & \Delta_{23} &= -a^{*1} - \left(d_{44}^{12} + d^{*1}\right)\xi^2 = \Delta_{32},\\
\Delta_{12} &= a^{**} - \left(c_{44}^{12} + c^{**}\right)\xi^2 = \Delta_{21}, & \Delta_{24} &= -a^{*2} - \left(d_{44}^{22} + d^{*2}\right)\xi^2 = \Delta_{42},\\
\Delta_{13} &= a^{*1} - \left(d_{44}^{11} - d^{*1}\right)\xi^2 = \Delta_{31}, & \Delta_{33} &= -a_{11}^{11} - \left(b_{44}^{11} + b_{77}^{11}\right)\xi^2,\\
\Delta_{14} &= a^{*2} - \left(d_{44}^{21} - d^{*2}\right)\xi^2 = \Delta_{41}, & \Delta_{34} &= -a_{11}^{12} - \left(b_{44}^{12} + b_{77}^{12}\right)\xi^2, = \Delta_{43}\\
\Delta_{22} &= \rho^{(2)}\omega^2 - a^{**} - \left(c_{44}^{22} - c^{**}\right)\xi^2, & \Delta_{44} &= -a_{11}^{22} - \left(b_{44}^{22} + b_{77}^{22}\right)\xi^2.
\end{aligned} \tag{12.45}$$

Again, this is a quartic in ξ^2 with two real branches. For the long wave behavior of the transverse acoustic branch:

$$\lim_{\omega,\xi\to 0} \Delta_T = \lim_{\omega,\xi\to 0} \left[(c_{44}^{11} + c_{44}^{22} + 2c_{44}^{12})\xi^2 - (\rho^{(1)}+\rho^{(2)})\omega^2 \right] D, \quad (12.46)$$

where

$$D = \begin{vmatrix} a_{11}^{11} & a_{11}^{12} & a^{*1} \\ a_{11}^{21} & a_{11}^{22} & a^{*2} \\ a^{*1} & a^{*2} & a^{**} \end{vmatrix}. \quad (12.47)$$

Hence, there is a transverse acoustic branch with limiting, low frequency behavior

$$\omega_{TA} = \xi\left[(c_{44}^{11} + c_{44}^{22} + 2c_{44}^{12})/(\rho^{(1)}+\rho^{(2)}) \right]^{1/2}. \quad (12.48)$$

The long wave limit of the transverse optical branch is found from

$$\lim_{\xi\to 0} \Delta_T = \omega^2 \left[\rho^{(1)}\rho^{(2)}\omega^2 (a_{11}^{11}a_{11}^{22} - a_{11}^{12}a_{11}^{21}) - (\rho^{(1)}+\rho^{(2)})D \right], \quad (12.49)$$

from which the limiting frequency of the transverse optical branch is

$$\omega_{TO} = \left[D/\bar{\rho}\,(a_{11}^{11}a_{11}^{22} + a_{11}^{12}a_{11}^{21}) \right]^{1/2}. \quad (12.50)$$

vi. One-dimensional NaCl-type Lattice of Shell-model Atoms.

The purpose of this section is to show that the one-dimensional equations of longitudinal motion (12.33) are the long wave limit of the difference equations of motion of a one-dimensional NaCl-type lattice of shell model atoms. Such a lattice is conveniently represented by two lines of alternating atoms (positive and negative ions, in the case of an ionic crystal) with one atom of each type at each lattice site, as shown in Fig. 19 — where the two types of atom are identified by the digits 1 and 2. Nearest neighbor interactions between unlike (adjacent) atoms in each line and next nearest neighbor interactions between like atoms in the two lines are those taken into account, but no interactions between unlike atoms at the

same site are considered. With each of p and q taking on the identifications 1 or 2, the force constants of the interactions are denoted by α_p for the intra-atomic core–shell interactions and $\beta_{pq}, \gamma_{pq}, \delta_{pq}$ for the core–core, core–shell and shell–shell interatomic interactions, respectively, between like atoms for $p = q$ and unlike atoms for $p \neq q$. We note that $\beta_{pq} = \beta_{qp}$ and $\delta_{pq} = \delta_{qp}$ but $\gamma_{pq} \neq \gamma_{qp}$. The two lines of atoms are taken to be parallel to the x_1 axis with the atom sites at $x_1 = na$, where n is a positive or negative integer. The displacements of the cores and shells of the atom at $x_1 = na$ are denoted by $u_n^{(\kappa)}$ and $s_n^{(\kappa)}$, respectively, where $\kappa = 1, 2$ to designate the atoms of types 1 and 2. (1 for the positive ion and 2 for the negative ion, in the case of an ionic crystal).

The equation of motion of the n^{th} atom of type 1 is obtained by equating its inertia force to the sum of the forces on its core and shell exerted by the cores and shells of the two nearest neighbor (unlike) atoms, the two next nearest neighbor (like) atoms and the Maxwell, electric self-field at $x_1 = na$:

$$\begin{aligned}
&\beta_{11}(u_{n+1}^{(1)} - u_n^{(1)}) + \gamma_{11}(s_{n+1}^{(1)} - s_n^{(1)} + u_{n+1}^{(1)} - u_n^{(1)}) + \delta_{11}(s_{n+1}^{(1)} - s_n^{(1)}) \\
&- \beta_{11}(u_n^{(1)} - u_{n-1}^{(1)}) - \gamma_{11}(u_n^{(1)} - u_{n-1}^{(1)} + s_n^{(1)} - s_{n-1}^{(1)}) - \delta_{11}(s_n^{(1)} - s_{n-1}^{(1)}) \\
&+ \beta_{12}(u_{n+1}^{(2)} - u_n^{(1)}) + \gamma_{12}(s_{n+1}^{(2)} - u_n^{(1)}) + \gamma_{21}(u_{n+1}^{(2)} - s_n^{(1)}) + \delta_{12}(s_{n+1}^{(2)} - s_n^{(1)}) \\
&- \beta_{12}(u_n^{(1)} - u_{n-1}^{(2)}) - \gamma_{12}(u_n^{(1)} - s_{n-1}^{(2)}) - \gamma_{21}(s_n^{(1)} - u_{n-1}^{(2)}) - \delta_{12}(s_n^{(1)} - s_{n-1}^{(2)}) - q_* E_n = m_1 \ddot{u}_n^{(1)} \,. \qquad (12.51)
\end{aligned}$$

Similarly, for the shell, alone, of the type 1 atom:

$$\begin{aligned}
&\alpha_1(u_n^{(1)} - s_n^{(1)}) + \gamma_{11}(u_{n+1}^{(1)} - s_n^{(1)}) + \delta_{11}(s_{n+1}^{(1)} - s_n^{(1)}) - \gamma_{11}(s_n^{(1)} - u_{n-1}^{(1)}) - \delta_{11}(s_n^{(1)} - s_{n-1}^{(1)}) \\
&\quad + \gamma_{21}(u_{n+1}^{(2)} - s_n^{(1)}) + \delta_{12}(s_{n+1}^{(2)} - s_n^{(1)}) - \gamma_{21}(s_n^{(1)} - u_{n-1}^{(2)}) - \delta_{12}(s_n^{(1)} - s_{n-1}^{(2)}) + q E_n = 0, \qquad (12.52)
\end{aligned}$$

where q is the electronic charge and the mass of the shell is neglected.

We adopt the following definitions of electronic polarization densities and mass densities:

$$P_n^{(\kappa)} = (s_n^{(\kappa)} - u_n^{(\kappa)}) q / a^3 \,, \quad \rho^{(\kappa)} = m_\kappa / a^3 \,, \quad \kappa = 1, 2 \qquad (12.53)$$

and also make the following identifications:

$$
\begin{aligned}
a_{11}^{11} &= (\alpha_1 + 2\gamma_{11} + 2\gamma_{21} + 2\delta_{12})a^3 q^{-2}, & b_{11}^{12} &= a_{11}^{12} a^2/2 = \delta_{12} a^5 q^{-2}, \\
b_{11}^{11} &= \delta_{11} a^5 q^{-2}, & c_{11}^{12} &= a^{**} a^2/2 = (\beta_{12} + \gamma_{12} + \gamma_{21} + \delta_{12})a^{-1}, \\
c_{11}^{11} &= (\beta_{11} + 2\gamma_{11} + \delta_{11})a^{-1}, & d_{11}^{21} &= a^{*2} a^2/2 = (\gamma_{12} + \delta_{12})a^2 q^{-1}, \\
d_{11}^{11} &= (\gamma_{11} + \delta_{11})a^2 q^{-1}, & d_{11}^{12} &= -a^{*1} a^2/2 = (\gamma_{21} + \delta_{12})a^2 q^{-1}.
\end{aligned}
\tag{12.54}
$$

Then (12.51) and (12.52) can be written as

$$c_{11}^{11}\Delta^2 u_n^{(1)} + c_{11}^{12}\Delta^2 u_n^{(2)} + d_{11}^{11}\Delta^2 P_n^{(1)} + d_{11}^{21}\Delta^2 P_n^{(2)} + a^{*1} P_n^{(1)} + a^{*2} P_n^{(2)} + a^{**}(u_n^{(2)} - u_n^{(1)}) - q_* E_n = \rho^{(1)} \ddot{u}_n^{(1)}, \tag{12.55}$$

$$d_{11}^{11}\Delta^2 u_n^{(1)} + d_{11}^{12}\Delta^2 u_n^{(2)} + b_{11}^{11}\Delta^2 P_n^{(1)} + b_{11}^{12}\Delta^2 P_n^{(2)} - a_{11}^{11} P_n^{(1)} - a_{11}^{12} P_n^{(2)} - a^{*1}(u_n^{(2)} - u_n^{(1)}) + E_n = 0, \tag{12.56}$$

where Δ^2 is, again, the second central difference divided by a^2.

In the same way, for the type 2 atom,

$$c_{11}^{21}\Delta^2 u_n^{(1)} + c_{11}^{22}\Delta^2 u_n^{(2)} + d_{11}^{12}\Delta^2 P_n^{(1)} + d_{11}^{22}\Delta^2 P_n^{(2)} - a^{*1} P_n^{(1)} - a^{*2} P_n^{(2)} - a^{**}(u_n^{(2)} - u_n^{(1)}) + q_* E_n = \rho^{(2)} \ddot{u}_n^{(2)}, \tag{12.57}$$

$$d_{11}^{21}\Delta^2 u_n^{(1)} + d_{11}^{22}\Delta^2 u_n^{(2)} + b_{11}^{21}\Delta^2 P_n^{(1)} + b_{11}^{22}\Delta^2 P_n^{(2)} - a_{11}^{21} P_n^{(1)} - a_{11}^{22} P_n^{(2)} - a^{*2}(u_n^{(2)} - u_n^{(1)}) + E_n = 0, \tag{12.58}$$

where, in addition to (12.54), we identify

$$
\begin{aligned}
a_{11}^{22} &= (\alpha_2 + 2\gamma_{22} + 2\gamma_{12} + 2\delta_{12})a^3 q^{-2}, & b_{11}^{22} &= \delta_{22} a^5 q^{-2}, \\
c_{11}^{22} &= (\beta_{22} + 2\gamma_{22} + \delta_{22})a^{-1}, & d_{11}^{22} &= (\gamma_{22} + \delta_{22})a^2 q^{-1}.
\end{aligned}
\tag{12.59}
$$

Also, as in Article 8, the charge equation may be written as

$$-\epsilon_0 \partial^- \partial^+ \varphi_n + \partial^-[P_n^{(1)} + P_n^{(2)} + q_*(u_n^{(2)} - u_n^{(1)})] = 0, \tag{12.60}$$

where ∂^+ and ∂^- are the Taylor series expansions of the derivative $\partial/\partial x_1$ in terms of forward and backward differences, respectively.

<u>In the long wave limit,</u>

$$
\begin{aligned}
&u_n^{(\kappa)} \to u_1^{(\kappa)}(x_1), \quad P_n^{(\kappa)} \to P_1^{(\kappa)}(x_1), \quad E_n \to E_1(x_1) = -\partial\varphi/\partial x_1 \\
&\qquad \Delta^2 f_n \to \partial^2 f(x_1)/\partial x_1^2, \quad \partial^\pm \to \partial/\partial x_1 .
\end{aligned}
\tag{12.61}
$$

Then (12.55), (12.57), (12.56) and (12.60), in that order, reduce to the

five equations (12.33) in the order given. Since the continuum equations are the long wave limit of the lattice equations, the two dispersion relations are ipso facto the same in the long wave limit.

It should be observed that, strictly speaking, the real segments of the optical branches, in the continuum approximation, have no valid role in cases where the optical and acoustic modes are coupled – as, for example in solutions of the equations for free boundary conditions. The frequencies of the two types of mode must be the same, when they are coupled; but, any frequency on a real segment of an optical branch is so high that the wave length of the acoustic branch, at that frequency, is too short to be within the range of validity of the continuum approximation. In such situations there is, in general, an upper limit of frequency, set by the wave length limitation of the acoustic branches, to which the solution is restricted.

However, there is an important exception. At frequencies close to ω_{LO} or ω_{TO}, the wave length of the optical branch is extremely long in comparison with that of the acoustic branch. In that case, the amplitude of the contribution of the acoustic part, to the coupled mode, is small in comparison with the amplitude contribution of the optical part; so that the error introduced by the inaccuracy of the acoustic branch is small. In fact, the acoustic branch may be discarded, then, without seriously affecting what remains — thus simplifying the equations of motion. The situation is analogous to that in the theory of thickness-shear and flexural vibrations of plates [65]. The thickness shear branch corresponds to the optical branch and the flexural branch corresponds to the acoustic branch. At frequencies near the cut-off frequency of the thickness-shear branch, the amplitude ratio of the flexural to the thickness-shear modes is small [65]. In that case, the flexural branch can be discarded entirely and a simpler equation of motion for the thickness-shear mode, alone, may be

written [66]

In the long wave, low frequency limit, we have, in addition to (12.61),

$$u_1^{(1)} = u_1^{(2)}, \quad P_1^{(1)} = P_1^{(2)}.$$

Then, with the notations

$$u_1 = u_1^{(1)} = u_1^{(2)}, \quad \tfrac{1}{2} P_1 = P_1^{(1)} = P_1^{(2)}, \quad \rho = \rho^{(1)} + \rho^{(2)},$$

$$a_{11} = \tfrac{1}{4}\left(a_{11}^{11} + a_{11}^{22} + 2a_{11}^{12}\right), \qquad b_{11} = \tfrac{1}{4}\left(b_{11}^{11} + b_{11}^{22} + 2\,b_{11}^{12}\right),$$

$$c_{11} = c_{11}^{11} + c_{11}^{22} + 2\,c_{11}^{12}, \qquad d_{11} = \tfrac{1}{2}\left(d_{11}^{11} + d_{11}^{22} + d_{11}^{12} + d_{11}^{21}\right),$$

the sum of (12.55) and (12.57), the sum of (12.56) and (12.58) and, finally, (12.60) become, respectively,

$$\begin{aligned} c_{11}u_{1,11} + d_{11}P_{1,11} &= \rho\ddot{u}_1 \\ d_{11}u_{1,11} + b_{11}P_{1,11} - a_{11}P_1 - \varphi_{,1} &= 0, \\ -\epsilon_0\varphi_{,11} + P_{1,1} &= 0. \end{aligned}$$

These are the equations (7.16) exhibited in Article 1 for longitudinal waves in a simple, as opposed to a compound, dielectric continuum, with symmetry m3m, when the polarization gradient is taken into account. Thus, the long wave limit of the equations of the one-dimensional, diatomic lattice yields the equations for longitudinal waves in the compound continuum when no restriction is placed on the frequency; whereas the long wave, low frequency limit yields the equations of the simple continuum.

At very low frequencies, the acoustic branch is nearly exact and, at zero frequency, it is absent. The quality of the approximation then depends on the low or zero frequency values of the imaginary or complex branches of the dispersion relation. These affect behavior at or near surfaces. A typical example is given by the difference between $i\ell$ and $i\lambda$, the imaginary wave lengths at zero frequency of the imaginary branches of the continuum and lattice dispersion relations, in Article 8, and the

role of this difference in the solutions of the continuum and lattice equations for capacitance of thin films, in Article 9.

13. Coupled Elastic and Electromagnetic Fields in a Diatomic, Dielectric Continuum

Equations governing coupled mechanical and electromagnetic fields in diatomic, ionic, optically isotropic crystals were given by Huang [67, 68] in terms of a polarization variable, the relative displacement of the ions and the usual variables of the electromagnetic field. These equations have been extended take into account the separate electronic polarizations and the separate displacements of the two ions, the ionic polarization, the two electronic polarization gradients and the two displacement gradients. Aside from a more detailed representation of the atomic and electronic interactions, there are two main effects of the additional considerations: first, the equations are applicable to shorter wave lengths, owing to the inclusion of the displacement and polarization gradients; second, the acoustic branches are included in the dispersion relations for plane waves, in addition to the optical branches and the electromagnetic branch.

As in Article 12, each of the two interpenetrating continua representing the diatomic crystal has its own displacement $u_i^{(\kappa)}$, $\kappa = 1, 2$, and electronic polarization $P_i^{(\kappa)}$. The stored energy of deformation and polarization is the same as before: a function of the individual small strains, $S_{ij}^{(\kappa)}$, the individual polarizations and polarization gradients, $P_i^{(\kappa)}$ and $P_{j,i}^{(\kappa)}$, and the relative displacement, u_i^* and rotation, ω_{ij}^*:

$$W^L = W^L\left(S_{ij}^{(1)}, S_{ij}^{(2)}, P_i^{(1)}, P_i^{(2)}, P_{j,i}^{(1)}, P_{j,i}^{(2)}, u_i^*, \omega_{ij}^*\right). \tag{13.1}$$

Also, as before, the total polarization, per unit area, P_i, is the sum of the electronic polarizations and the ionic polarization:

$$P_i = P_i^{(1)} + P_i^{(2)} + q_* u_i^* . \tag{13.2}$$

Of the variables in (13.1), only P_i and u_i^* are accounted for in Huang's [67, 68] equations of motion.

When the Maxwell, electric self-field, E_i, is quasi-static, it satisfies

$$\delta_{ijk} E_{k,j} = 0, \tag{13.3}$$

where, as in (3.2), δ_{ijk} is the unit alternating tensor. In the electromagnetic case, (13.3) is replaced by

$$\delta_{ijk} E_{k,j} + \dot{B}_i = 0, \tag{13.4}$$

where, as in Article 11, the magnetic flux density, B_i, satisfies

$$\mu_0^{-1} \delta_{ijk} B_{k,j} = \epsilon_0 \dot{E}_i + \dot{P}_i, \quad B_{i,i} = 0. \tag{13.5}$$

In addition to (13.4) and (13.5) the field equations (12.31) also hold, but with $\varphi_{,i}$ replaced by $-E_i$.

Plane waves in the [100] direction are expressed by

$$u_i^{(k)} = K_i^{(k)} e^{i\psi}, \quad P_i^{(k)} = L_i^{(k)} e^{i\psi}, \quad E_i = M_i e^{i\psi}, \quad B_i = N_i e^{i\psi} \tag{13.6}$$

where $\psi = \xi x_1 - \omega t$ and $K_i^{(k)}$, $L_i^{(k)}$, M_i and N_i are constants.

In the case of longitudinal waves,

$$u_2^{(k)} = u_3^{(k)} = 0, \quad P_2^{(k)} = P_3^{(k)} = 0, \quad E_2 = E_3 = 0, \tag{13.7}$$

$$u_1^{(k)} = K_1^{(k)} e^{i\psi}, \quad P_1^{(k)} = L_1^{(k)} e^{i\psi}, \quad E_1 = M_1 e^{i\psi}. \tag{13.8}$$

Then, from (13.4), $B_i = 0$; i.e. there is no coupling with the magnetic field. However the Maxwell, electric self-field is coupled with the displacement and polarization fields. The solution, therefore, is the same as that found in Article 12 for the case of the quasi-static electric field, with dispersion relation (12.35) as the result.

Of the two similar transverse waves, with displacements in the directions of x_2 and x_3, we choose the former for examination:

$$u_1^{(k)} = u_3^{(k)} = 0, \quad P_1^{(k)} = P_3^{(k)} = 0, \quad E_1 = E_3 = 0, \quad B_1 = B_2 = \ , \tag{13.9}$$

$$u_2^{(k)} = K_2^{(k)} e^{i\psi}, \quad P_2^{(k)} = L_2^{(k)} e^{i\psi}, \quad E_2 = M_2 e^{i\psi}, \quad B_3 = N_3 e^{i\psi}. \tag{13.10}$$

In the case of the quasi-static electric field, the absence of (13.5) permitted E_2, as well as B_3, to be zero; but both must be non-zero when the full electromagnetic equations are imposed.

To find a form of the dispersion determinant similar to (12.44), it is useful first to express M_2 and N_3 in terms of $K_2^{(\kappa)}$ and $L_2^{(\kappa)}$ through the use of (13.4) and (13.5):

$$M_2 = -i\omega N_3 \xi^{-1} = -\epsilon_\xi^{-1}\left[L_2^{(1)} + L_2^{(2)} + q_*(K_2^{(2)} - K_2^{(1)})\right], \tag{13.11}$$

where

$$\epsilon_\xi = \epsilon_0 - \xi^2/\mu_0\omega^2. \tag{13.12}$$

When the results (13.11), along with (13.9) and (13.10), are inserted in the remaining equations of motion, the latter are satisfied if

$$\Delta_T^{EM} = 0, \tag{13.13}$$

where Δ_T^{EM} is the determinant with elements

$$\begin{aligned}
\Delta_{11} &= \rho^{(1)}\omega^2 - a^{**} - q_*\epsilon_\xi^{-1} - (c_{44}^{11} - c^{**})\xi^2, \\
\Delta_{12} &= a^{**} + q_*^2\epsilon_\xi^{-1} - (c_{44}^{21} + c^{**})\xi^2 = \Delta_{21}, \\
\Delta_{13} &= a^{*1} + q_*\epsilon_\xi^{-1} - (d_{44}^{11} - d^{*1})\xi^2 = \Delta_{31}, \\
\Delta_{14} &= a^{*2} + q_*\epsilon_\xi^{-1} - (d_{44}^{21} - d^{*2})\xi^2 = \Delta_{41}, \\
\Delta_{22} &= \rho^{(2)}\omega^2 - a^{**} - q_*^2\epsilon_\xi^{-1} - (c_{44}^{22} - c^{**})\xi^2,
\end{aligned}
\qquad
\begin{aligned}
\Delta_{23} &= -a^{*1} - q_*\epsilon_\xi^{-1} - (d_{44}^{12} + d^{*1})\xi^2 = \Delta_{32}, \\
\Delta_{24} &= -a^{*2} - q_*\epsilon_\xi^{-1} - (d_{44}^{22} + d^{*2})\xi^2 = \Delta_{42}, \\
\Delta_{33} &= -a_{11}^{11} - \epsilon_\xi^{-1} - (b_{44}^{11} + b_{77}^{11})\xi^2, \\
\Delta_{34} &= -a_{11}^{21} - \epsilon_\xi^{-1} - (b_{44}^{21} + b_{77}^{21})\xi^2 = \Delta_{43}, \\
\Delta_{44} &= -a_{11}^{22} - \epsilon_\xi^{-1} - (b_{44}^{22} + b_{77}^{22})\xi^2.
\end{aligned}$$

The long wave, high frequency behavior is obtained from

$$\lim_{\xi \to 0} \Delta_T^{EM} = \omega^4\left\{\rho^{(1)}\rho^{(2)}\omega^2\left[(a_{11}^{11} + \epsilon_0^{-1})(a_{11}^{22} + \epsilon_0^{-1}) - (a_{11}^{12} + \epsilon_0^{-1})^2\right] - (\rho^{(1)} + \rho^{(2)})D_L\right\}, \tag{13.14}$$

where D_L is again given by (12.38). Thus, the limiting frequency is

$$\omega_{TO}^{EM} = \left\{D_L/\bar{\rho}\left[(a_{11}^{11} + \epsilon_0^{-1})(a_{11}^{22} + \epsilon_0^{-1}) - (a_{11}^{12} + \epsilon_0^{-1})^2\right]\right\}^{1/2}, \tag{13.15}$$

i.e., as found by Huang [67, 68], the same as the limiting frequency of the longitudinal optical branch.

The long wave, low frequency behavior is given by

$$\lim_{\omega,\xi\to 0} \Delta_T^{EM} = \lim_{\omega,\xi\to 0} [(c_{44}^{11} + c_{44}^{22} + 2c_{44}^{12})\xi^2 - (\rho^{(1)} + \rho^{(2)})\omega^2] D_\xi, \tag{13.16}$$

where

$$D_\xi = (\epsilon_0\mu_0 D_L \omega^2 - \xi^2 D)/(\epsilon_0\mu_0\omega^2 - \xi^2) \tag{13.17}$$

and D is again given by (12.47). Thus, there are two branches, with limiting, low frequency, long wave behaviors

$$\omega_{EM} = \xi(D/\epsilon_0\mu_0 D_L)^{1/2}, \tag{13.18}$$

$$\omega_{TA}^{EM} = \xi[(c_{44}^{11} + c_{44}^{22} + 2c_{44}^{12})/(\rho^{(1)} + \rho^{(2)})]^{1/2}. \tag{13.19}$$

The first of these is the long wave end of the electromagnetic branch, with slope equal to the product of the velocity of electromagnetic waves in a vacuum $(\epsilon_0\mu_0)^{-1/2}$ and the index of refraction $(D_L/D)^{1/2}$ in the dielectric. The second is the long wave end of the transverse acoustic branch: identical with that for the quasi-static electric field (Article 12) and the purely elastic field (Article 4). The long wave portions of the real branches of the dispersion relations for both the longitudinal and transverse waves are illustrated in Fig. 20. The vertical scale of the acoustic branches is expanded: the ratio of their slopes to that of the electromagnetic branch is of the order of 10^{-5}.

The long wave behaviors of all the real branches are independent of the constants b_{ijkl}, c_{ijkl} and d_{ijkl}, i.e. independent of the polarization and displacement gradients. Also, the long wave limits of the acoustic branches depend only on the mass densities and the elastic stiffnesses. Hence, as far as the limiting behavior at the long wave end is concerned, the results, here, conform with Huang's, with the addition of the acoustic branches. However, as may be seen from the determinants (12.35) and (13.13), when the wave length diminishes from infinity, the displacement and polarization gradients affect the dispersion relation, as

does the coupling with the elastic field. Then the results diverge from Huang's.

A very general treatment, including crystals of arbitrary symmetry, an arbitrary number of ions and electrons per unit cell and non-linear, as well as linear, interactions, is given by Lax and Nelson [70].

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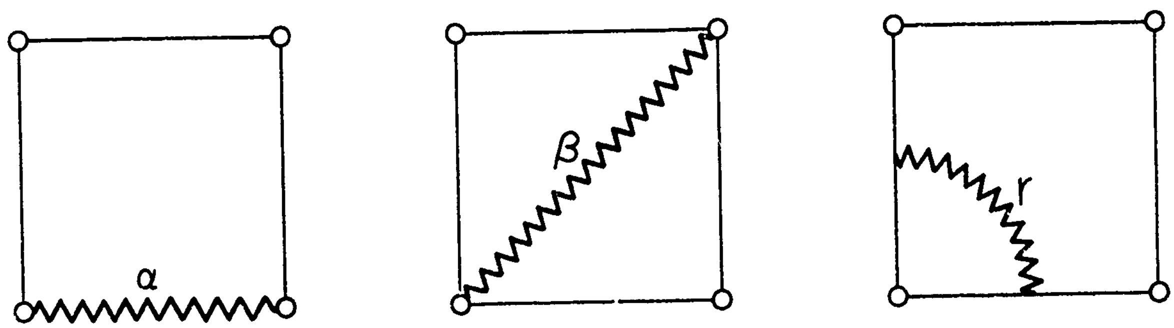


Fig. 1

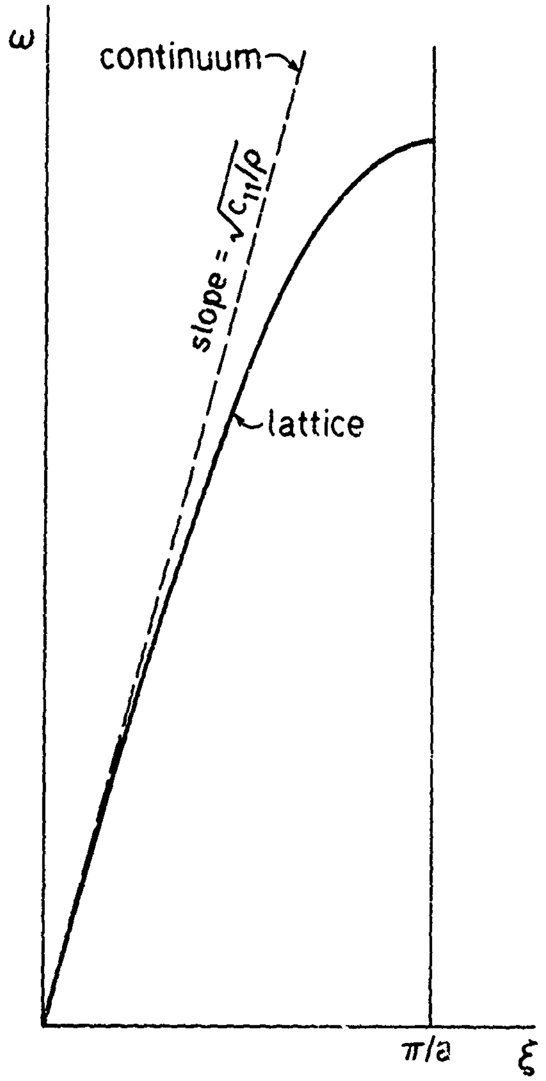


Fig. 2

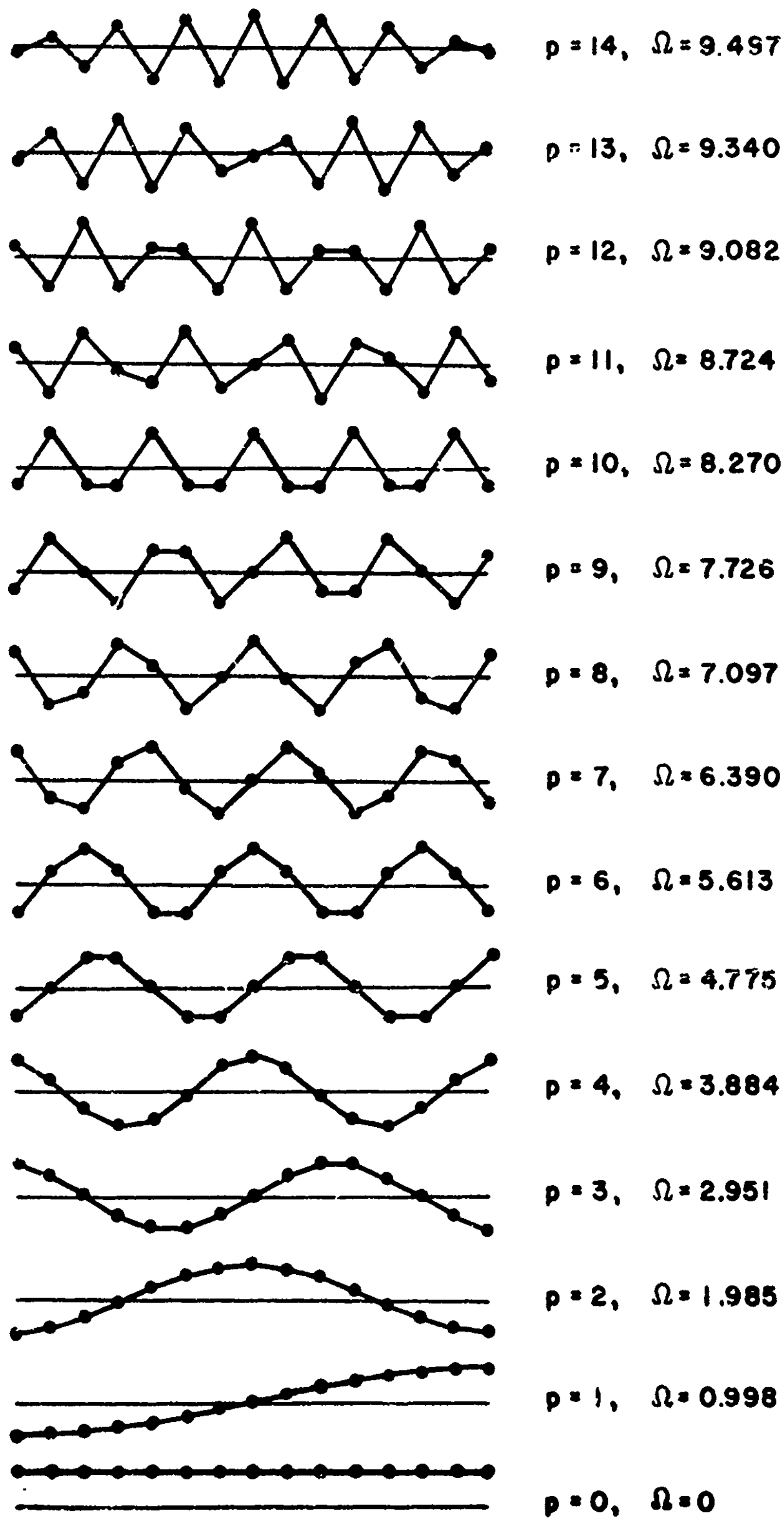

p = 14, Ω = 9.497
p = 13, Ω = 9.340
p = 12, Ω = 9.082
p = 11, Ω = 8.724
p = 10, Ω = 8.270
p = 9, Ω = 7.726
p = 8, Ω = 7.097
p = 7, Ω = 6.390
p = 6, Ω = 5.613
p = 5, Ω = 4.775
p = 4, Ω = 3.884
p = 3, Ω = 2.951
p = 2, Ω = 1.985
p = 1, Ω = 0.998
p = 0, Ω = 0

Fig. 3

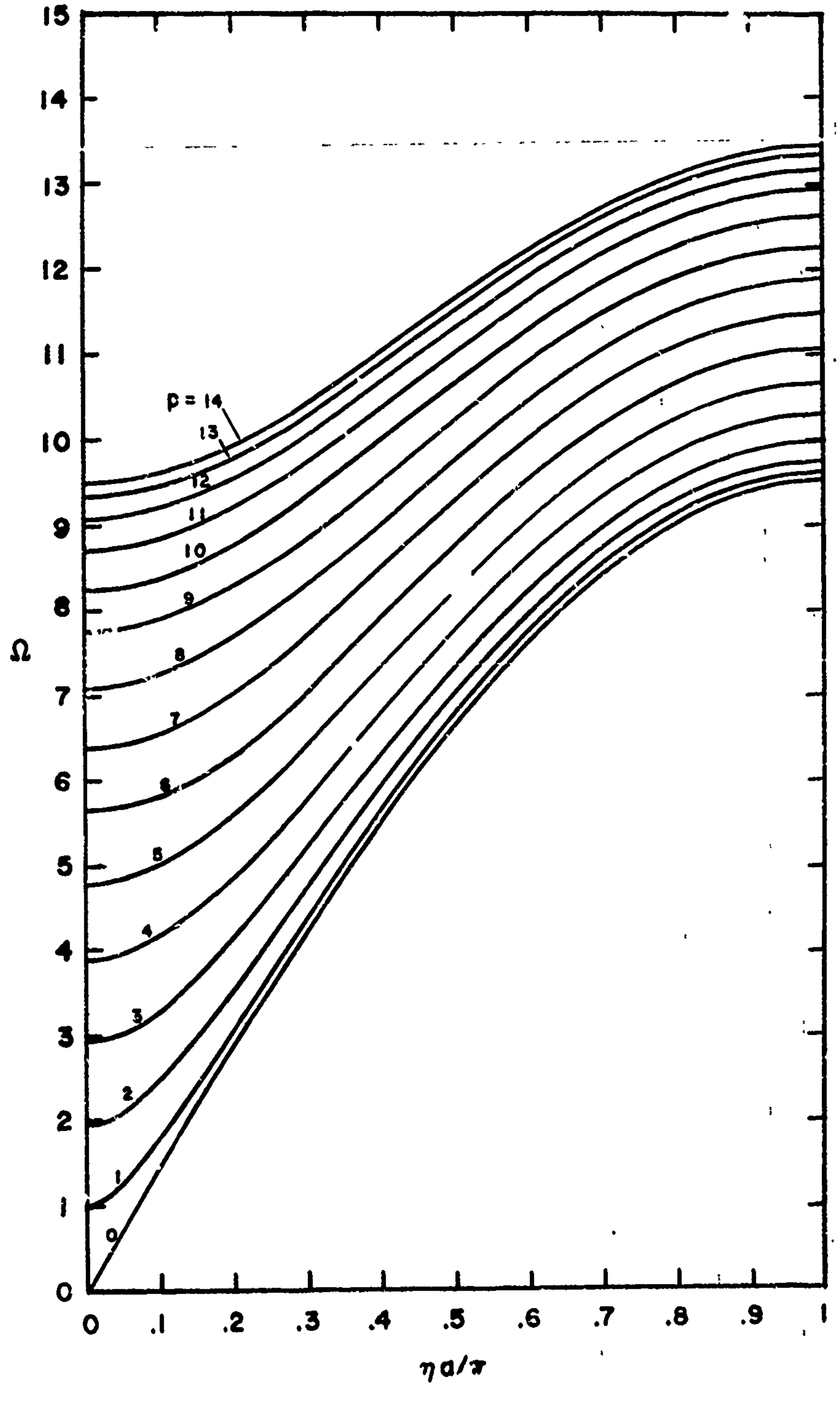
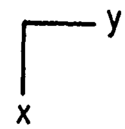

p = 14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
Ω
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
ηa/π

Fig.4

$$\begin{array}{ccc} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array} \qquad L = 1, \; M = 1$$



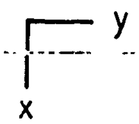
$$\begin{array}{ccccc} \frac{4}{5} & \frac{3}{5} & 0 & -\frac{3}{5} & -\frac{4}{5} \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{4}{5} & -\frac{3}{5} & 0 & \frac{3}{5} & \frac{4}{5} \end{array} \qquad L = 1, \; M = 2$$

$$\begin{array}{ccccccc} \frac{23}{13} & \frac{20}{13} & \frac{11}{13} & 0 & -\frac{11}{13} & -\frac{20}{13} & -\frac{23}{13} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{23}{13} & -\frac{20}{13} & -\frac{11}{13} & 0 & \frac{11}{13} & \frac{20}{13} & \frac{23}{13} \end{array} \qquad L = 1, \; M = 3$$

$$\begin{array}{ccccccccc} \frac{47}{17} & \frac{43}{17} & \frac{31}{17} & \frac{16}{17} & 0 & -\frac{16}{17} & -\frac{31}{17} & -\frac{43}{17} & -\frac{47}{17} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{47}{17} & -\frac{43}{17} & -\frac{31}{17} & -\frac{16}{17} & 0 & \frac{16}{17} & \frac{31}{17} & \frac{43}{17} & \frac{47}{17} \end{array} \qquad L = 1, \; M = 4$$

Fig. 5a

$$\begin{matrix} 0 & \frac{1}{3} & 0 & -\frac{1}{3} & 0 \\ -\frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 & -\frac{1}{3} \\ 0 & -\frac{1}{3} & 0 & \frac{1}{3} & 0 \end{matrix} \qquad L = 2,\ M = 2$$



$$\begin{matrix} \frac{448}{281} & \frac{498}{281} & \frac{300}{281} & 0 & -\frac{300}{281} & -\frac{498}{281} & -\frac{448}{281} \\ \frac{117}{281} & \frac{184}{281} & \frac{121}{281} & 0 & -\frac{121}{281} & -\frac{184}{281} & -\frac{117}{281} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{117}{281} & -\frac{184}{281} & -\frac{121}{281} & 0 & \frac{121}{281} & \frac{184}{281} & \frac{117}{281} \\ -\frac{448}{281} & -\frac{498}{281} & -\frac{300}{281} & 0 & \frac{300}{281} & \frac{498}{281} & \frac{448}{281} \end{matrix} \qquad L = 2,\ M = 3$$

$$\begin{matrix} \frac{7788}{2245} & \frac{8080}{2245} & \frac{6242}{2245} & \frac{3342}{2245} & 0 & -\frac{3342}{2245} & -\frac{6242}{2245} & -\frac{8080}{2245} & -\frac{7788}{2245} \\ \frac{3006}{2245} & \frac{3475}{2245} & \frac{2814}{2245} & \frac{1539}{2245} & 0 & -\frac{1539}{2245} & -\frac{2814}{2245} & -\frac{3475}{2245} & -\frac{3006}{2245} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3006}{2245} & -\frac{3475}{2245} & -\frac{2814}{2245} & -\frac{1539}{2245} & 0 & \frac{1539}{2245} & \frac{2814}{2245} & \frac{3475}{2245} & \frac{3006}{2245} \\ -\frac{7788}{2245} & -\frac{8080}{2245} & -\frac{6242}{2245} & -\frac{3342}{2245} & 0 & \frac{3342}{2245} & \frac{6242}{2245} & \frac{8080}{2245} & \frac{7788}{2245} \end{matrix} \qquad L = 2,\ M = 4$$

Fig. 5b

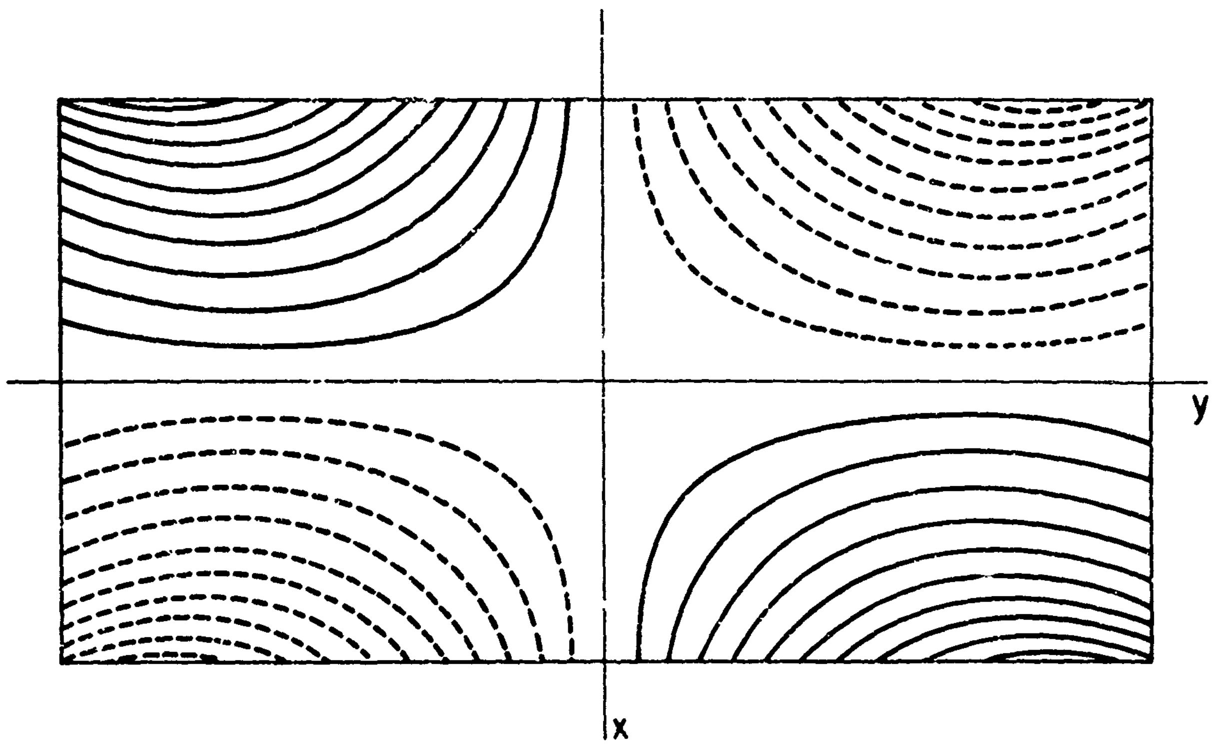


Fig. 6a

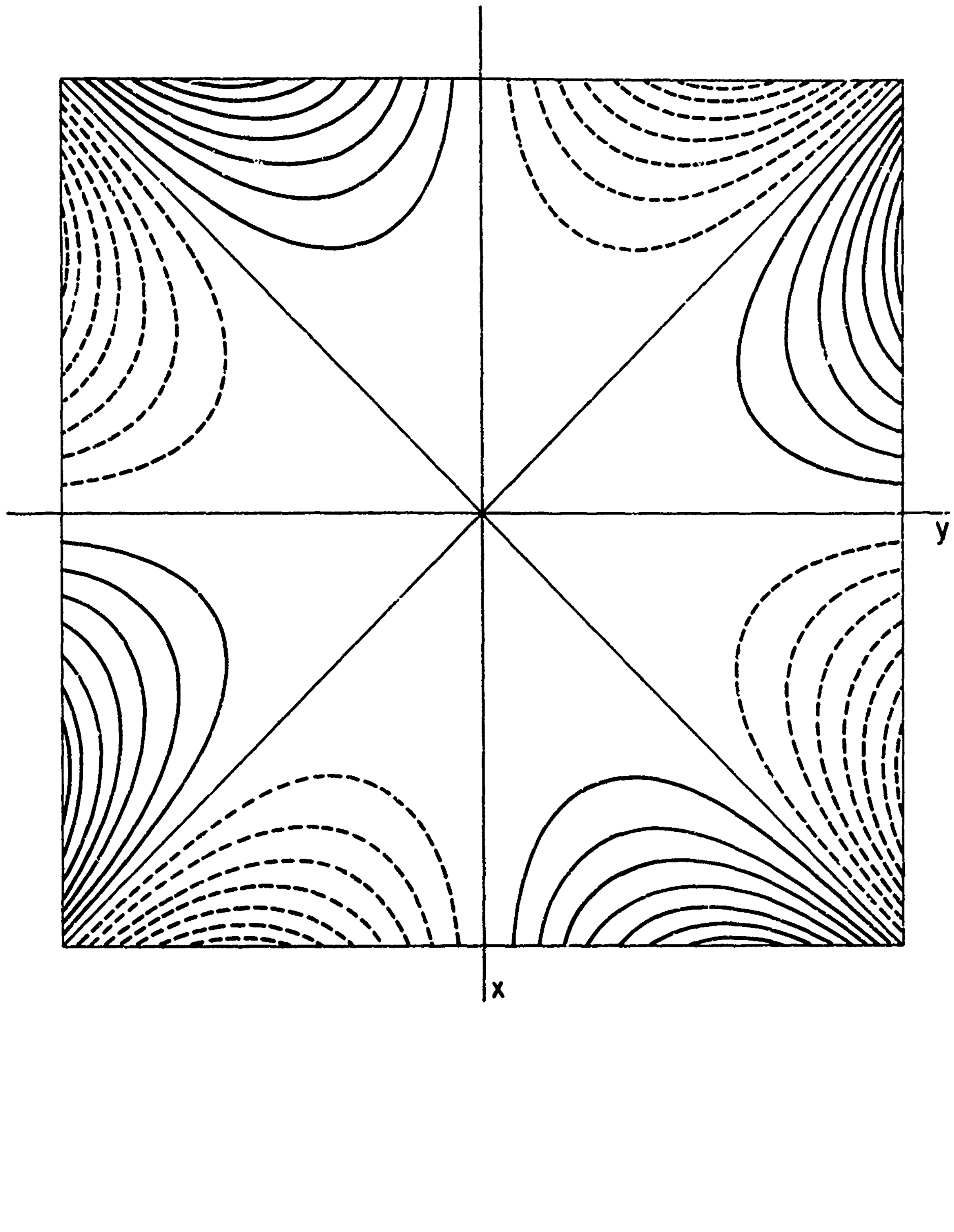


Fig. 6 b

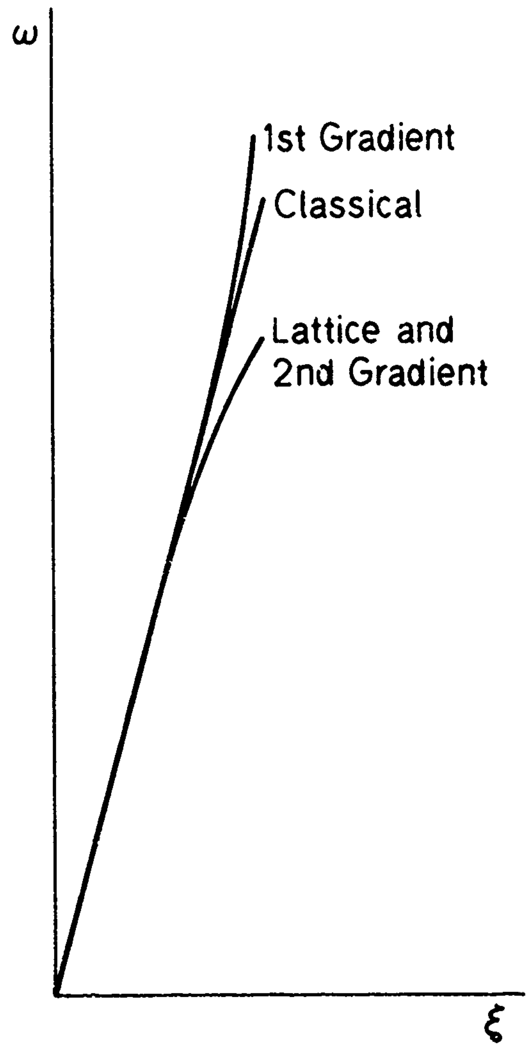


Fig.7

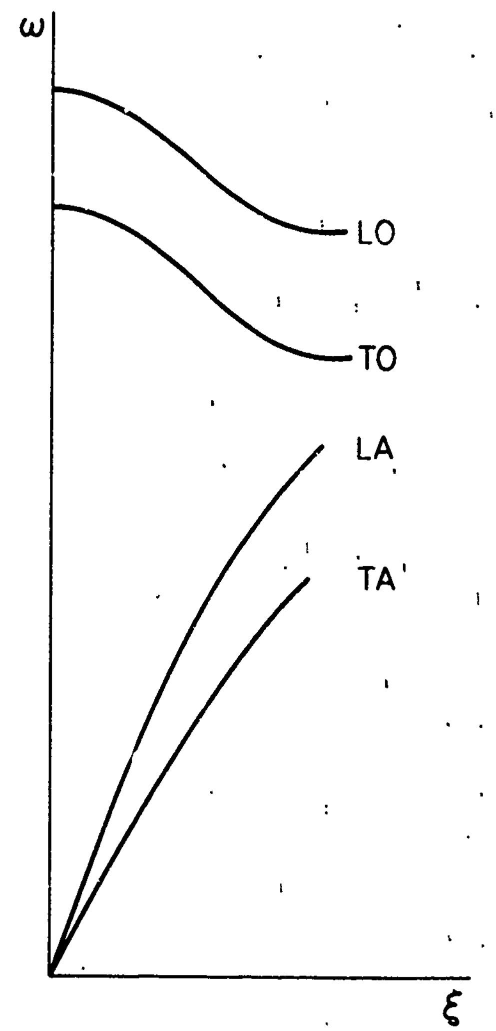


Fig. 8

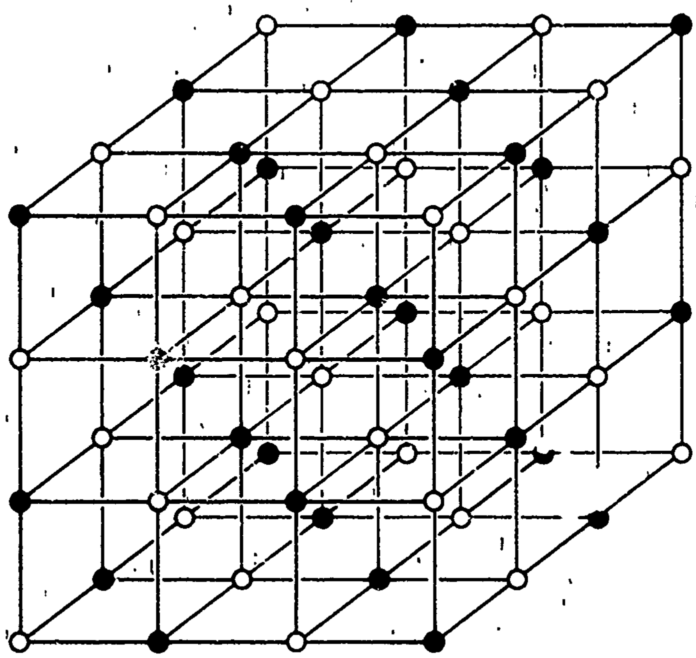


Fig. 9

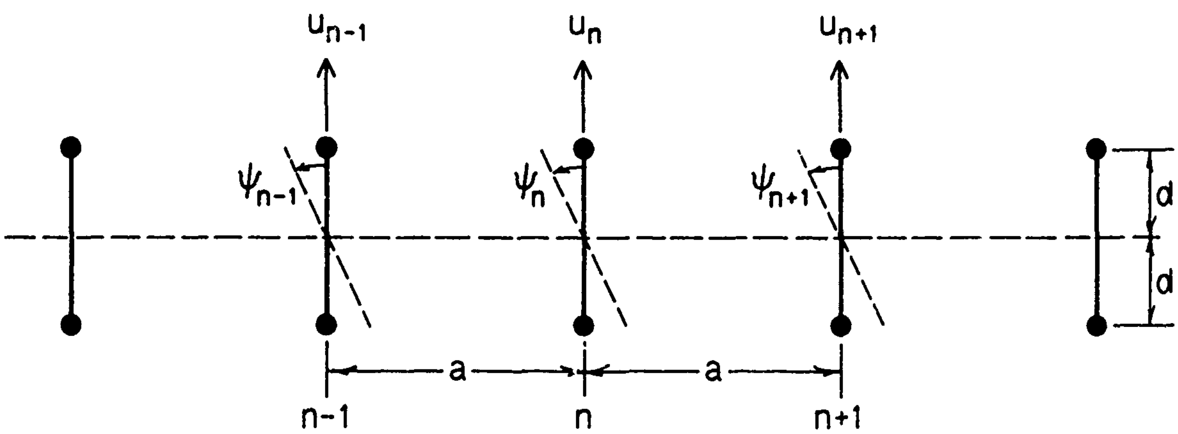


Fig. 10

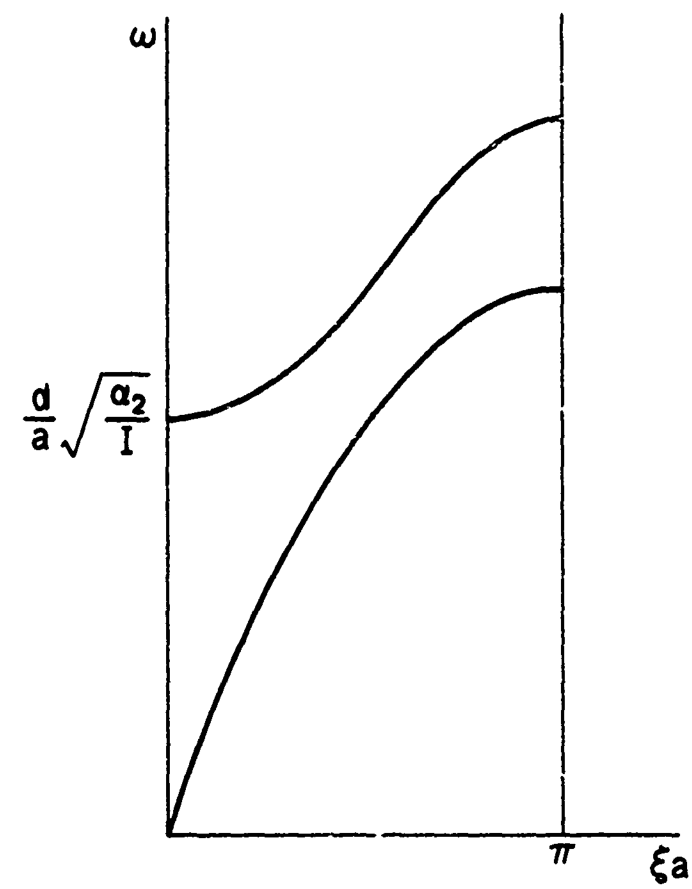


Fig. 11

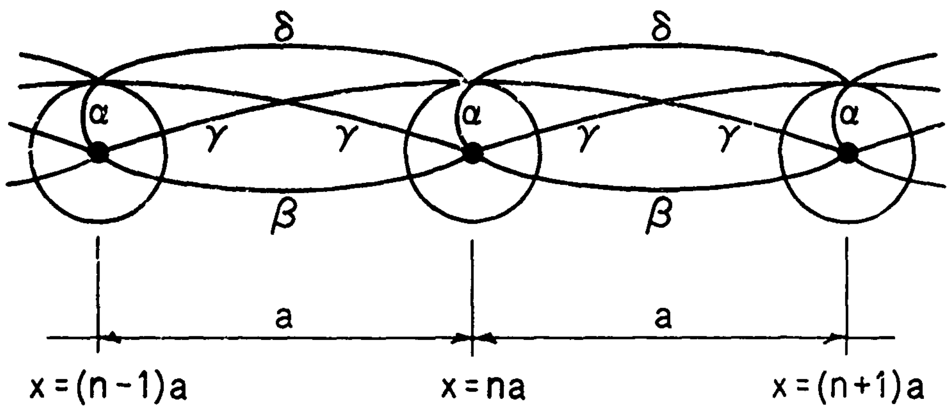


Fig. 12

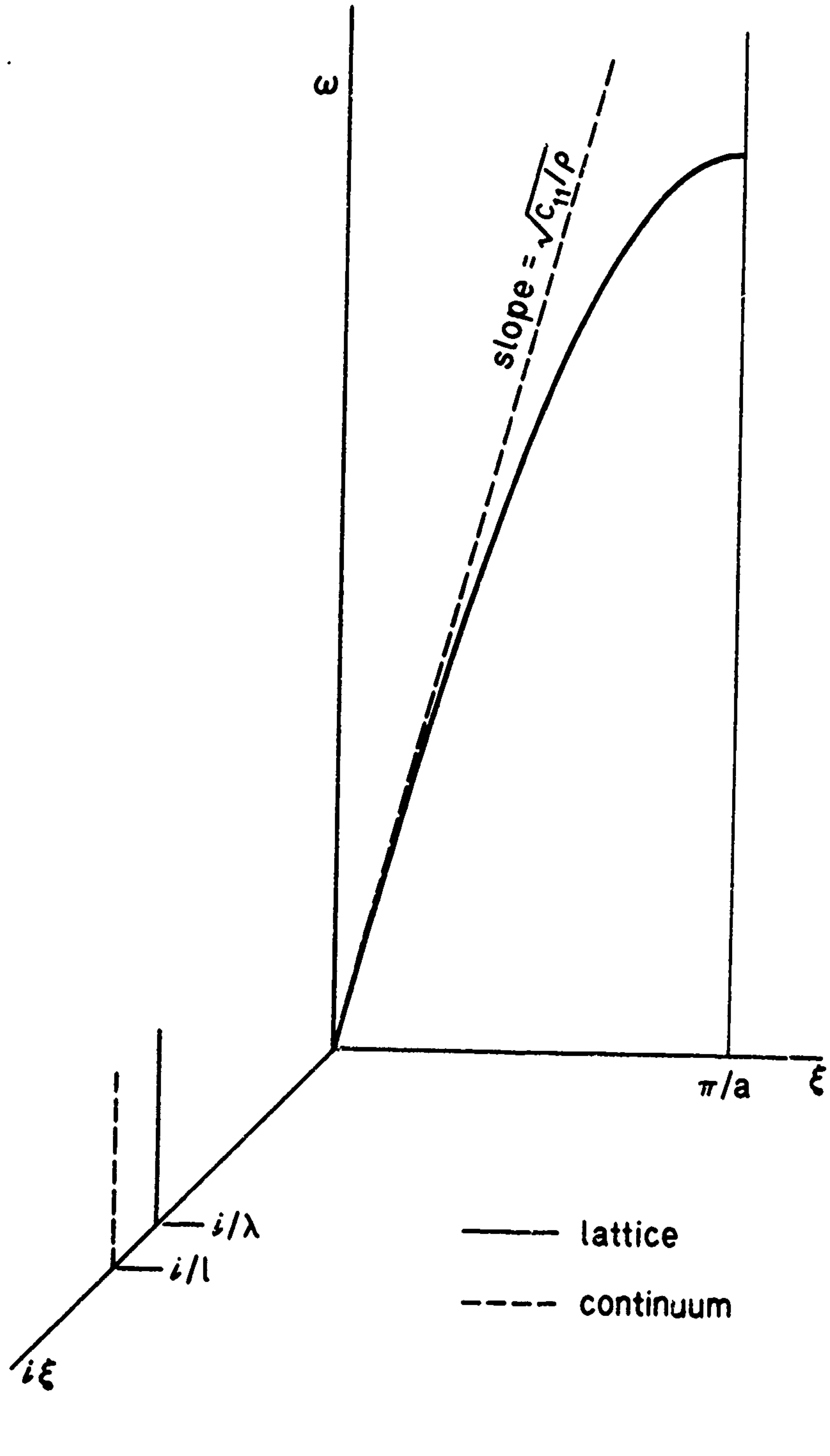


Fig.13

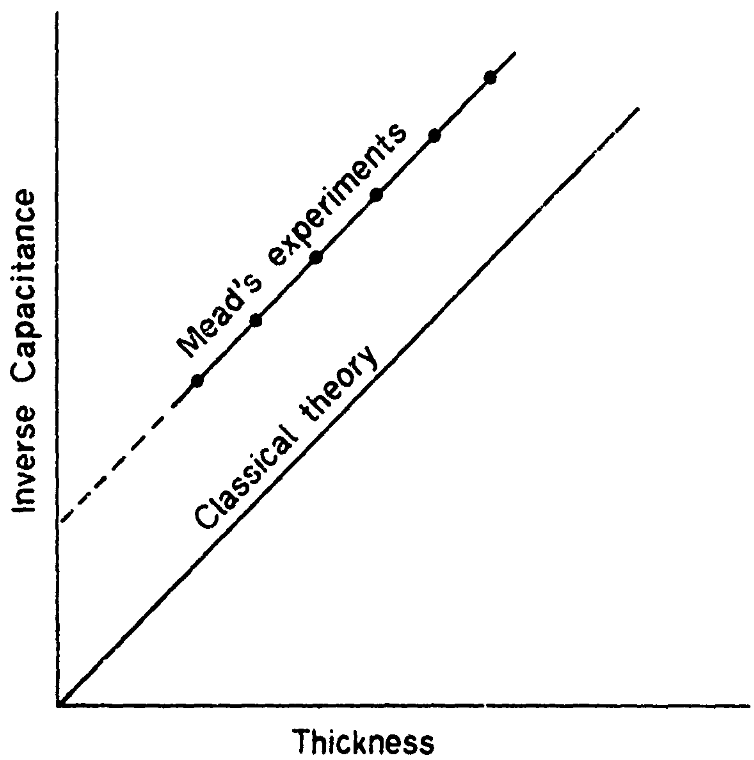
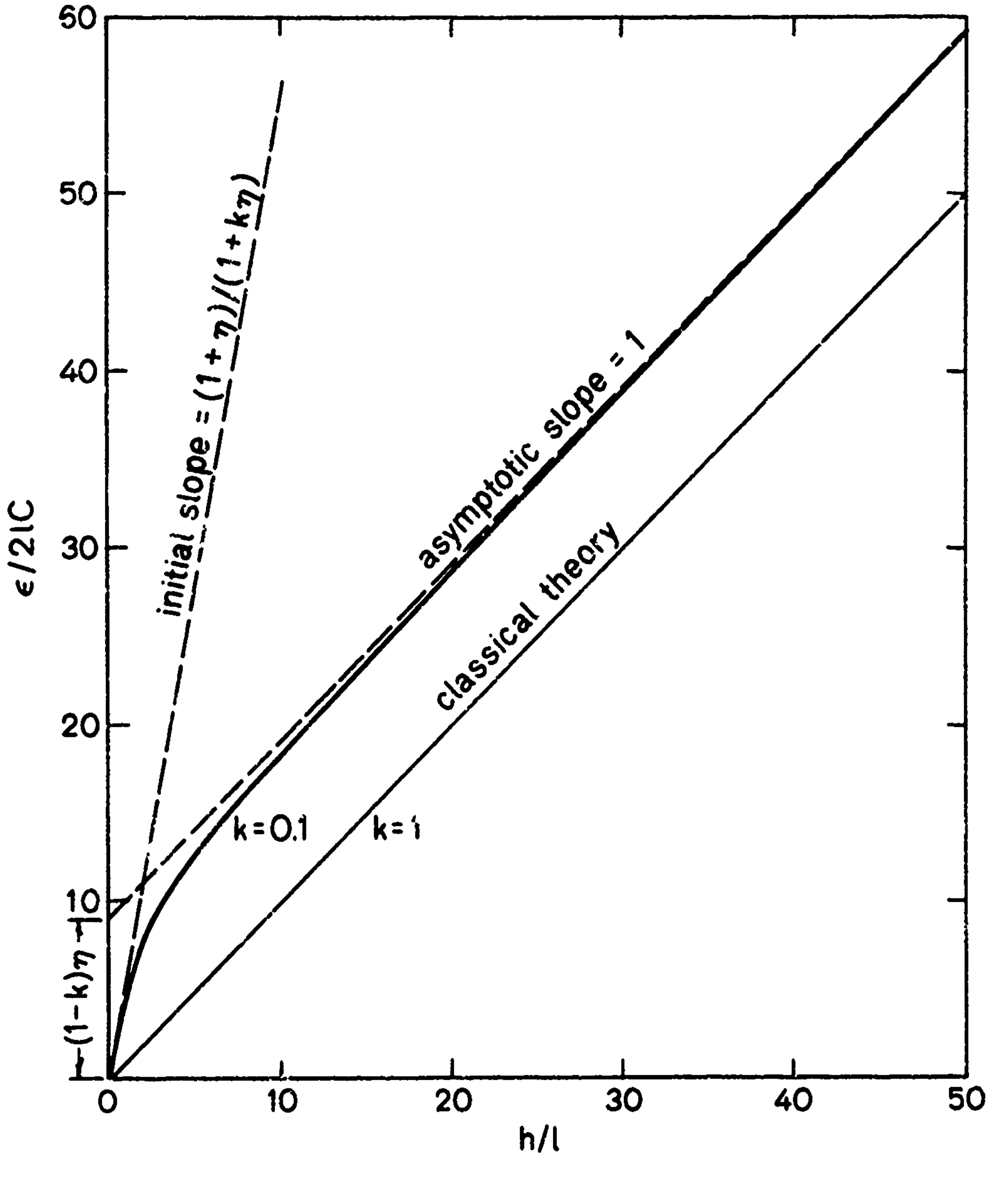

Inverse Capacitance
Mead's experiments
Classical theory
Thickness

Fig. 14



60
50
40
30
20
10
0
$(1-k)\eta$
10
20
30
40
50
$\epsilon/2lC$
h/l
initial slope = $(1+\eta)/(1+k\eta)$
asymptotic slope = 1
classical theory
k=0.1
k=1

Fig. 15

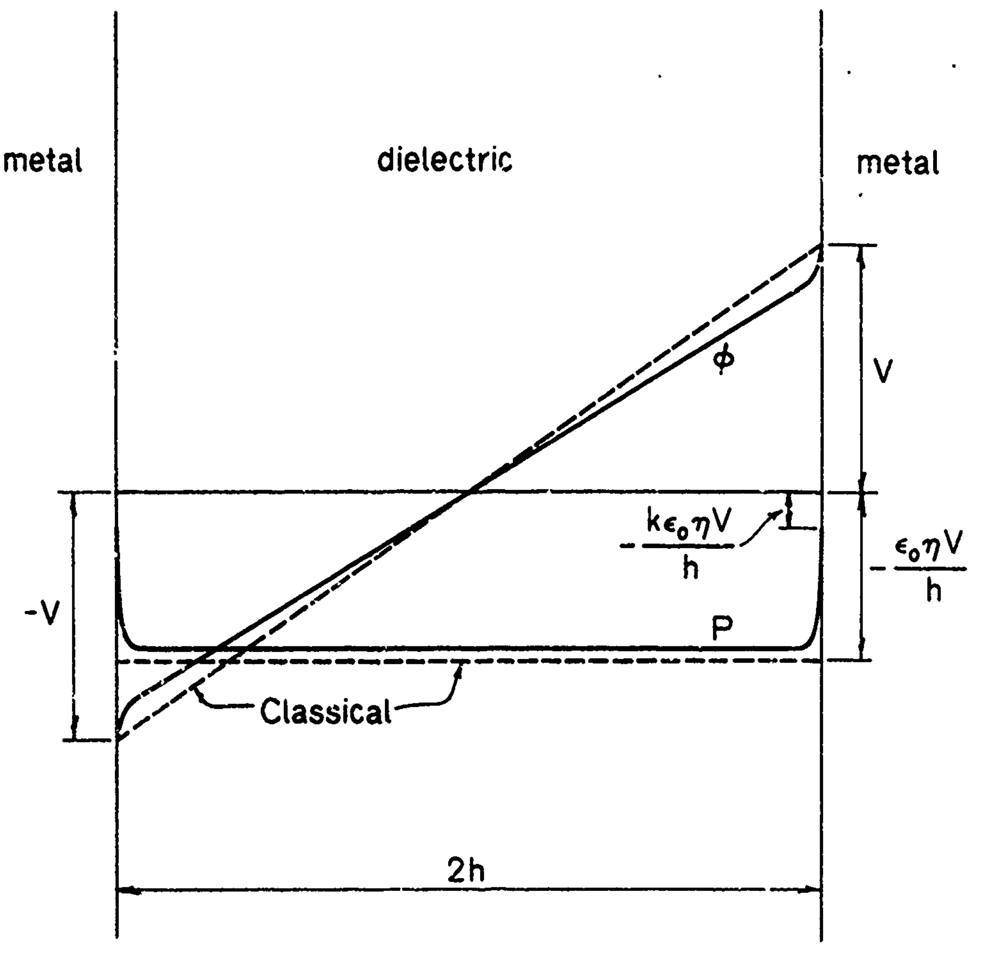

metal
dielectric
metal
V
ϕ
$-\frac{k\epsilon_0\eta V}{h}$
$-\frac{\epsilon_0\eta V}{h}$
-V
P
Classical
2h

Fig.16

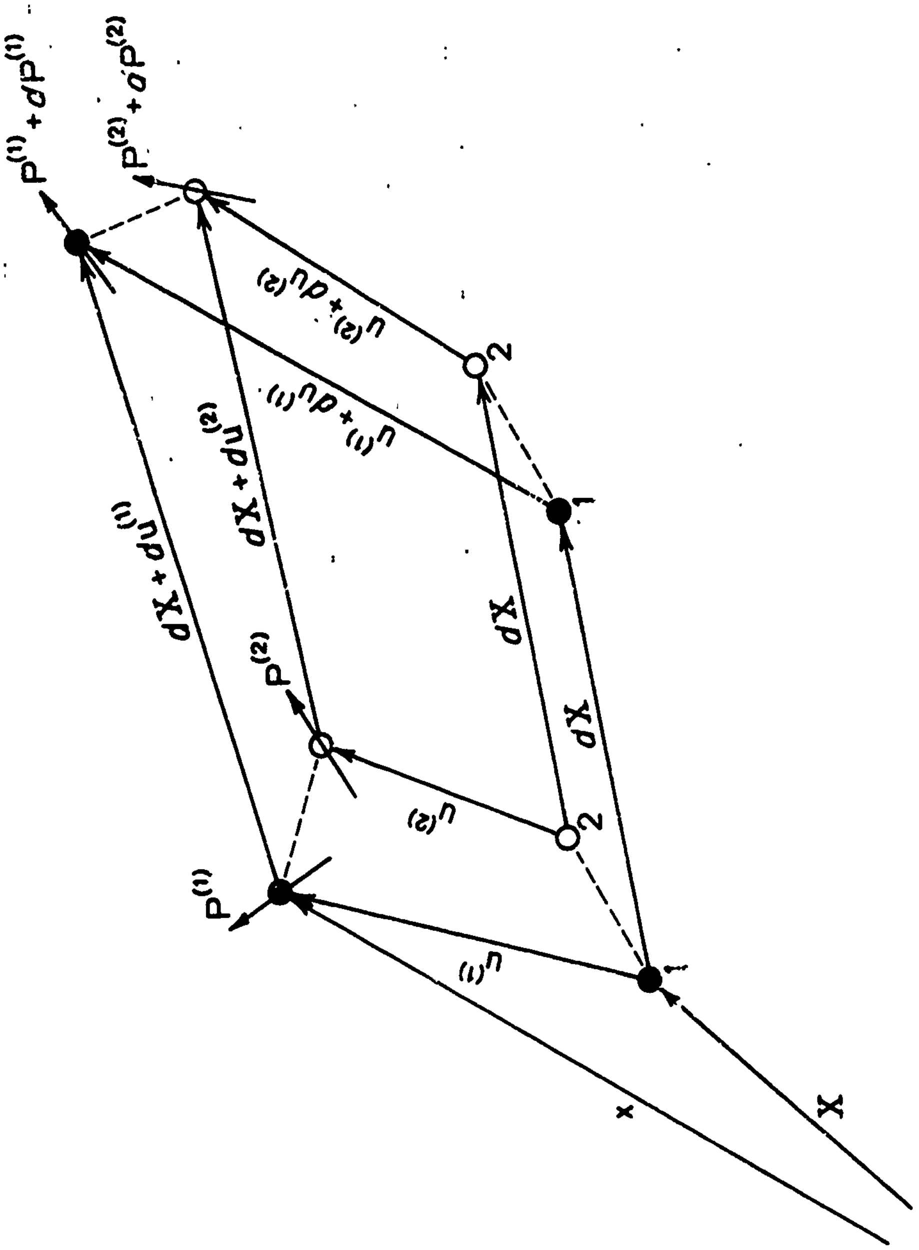
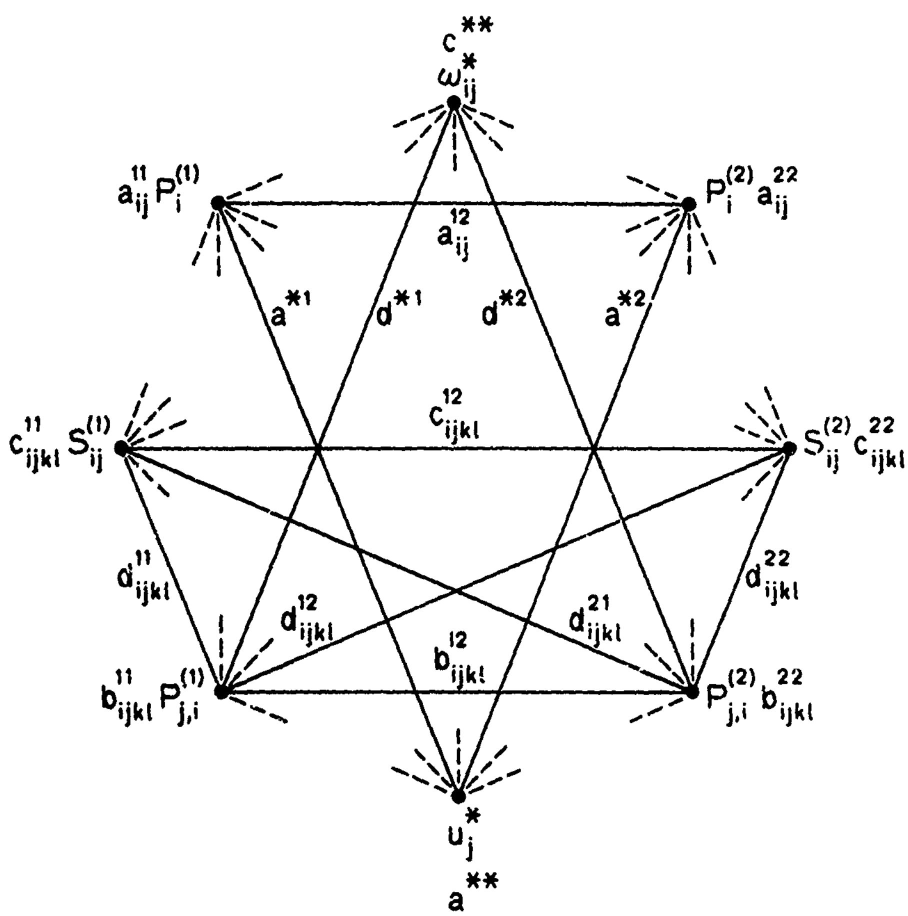
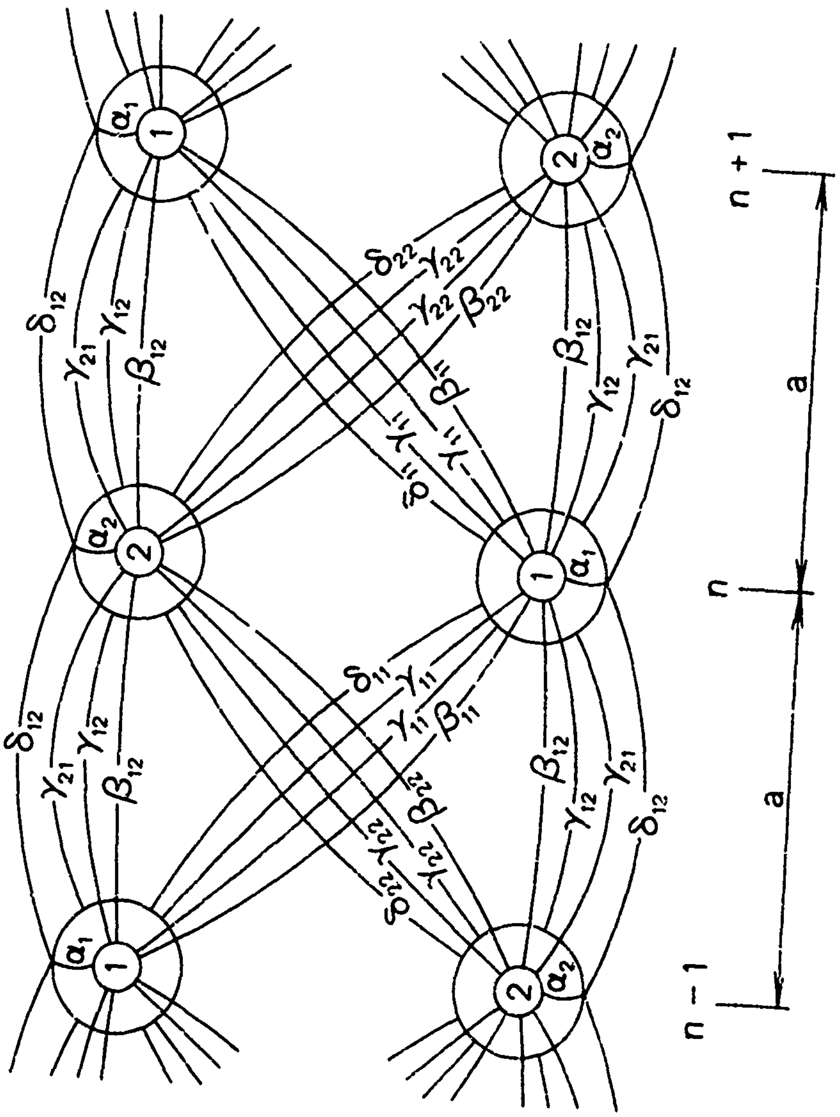


Fig. 17



c^{**}
ω^*_{ij}
$a^{11}_{ij}\ P^{(1)}_i$
$P^{(2)}_i\ a^{22}_{ij}$
a^{12}_{ij}
a^{*1}
d^{*1}
d^{*2}
a^{*2}
c^{12}_{ijkl}
$c^{11}_{ijkl}\ S^{(1)}_{ij}$
$S^{(2)}_{ij}\ c^{22}_{ijkl}$
d^{11}_{ijkl}
d^{12}_{ijkl}
d^{21}_{ijkl}
d^{22}_{ijkl}
b^{12}_{ijkl}
$b^{11}_{ijkl}\ P^{(1)}_{j,i}$
$P^{(2)}_{j,i}\ b^{22}_{ijkl}$
u^*_j
a^{**}

Fig.18



α_1
α_2
1
2
β_{12}
γ_{12}
γ_{21}
δ_{12}
β_{11}
γ_{11}
δ_{11}
β_{22}
γ_{22}
δ_{22}
a
a
n − 1
n
n + 1

Fig. 19

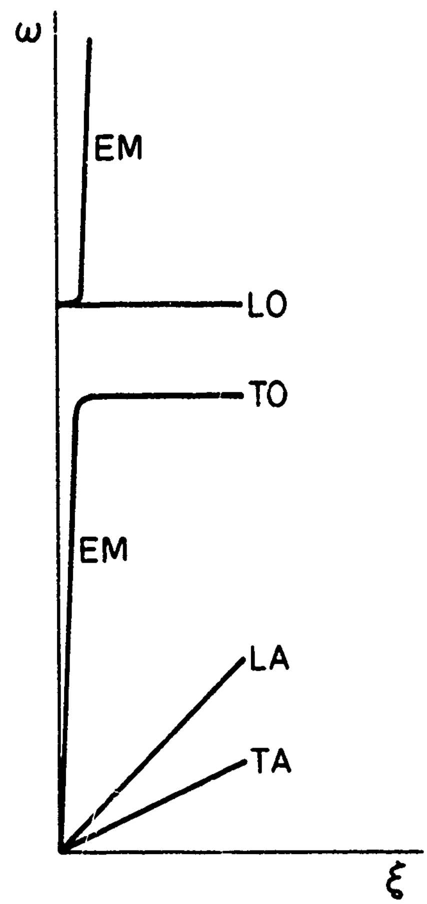


Fig. 20

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